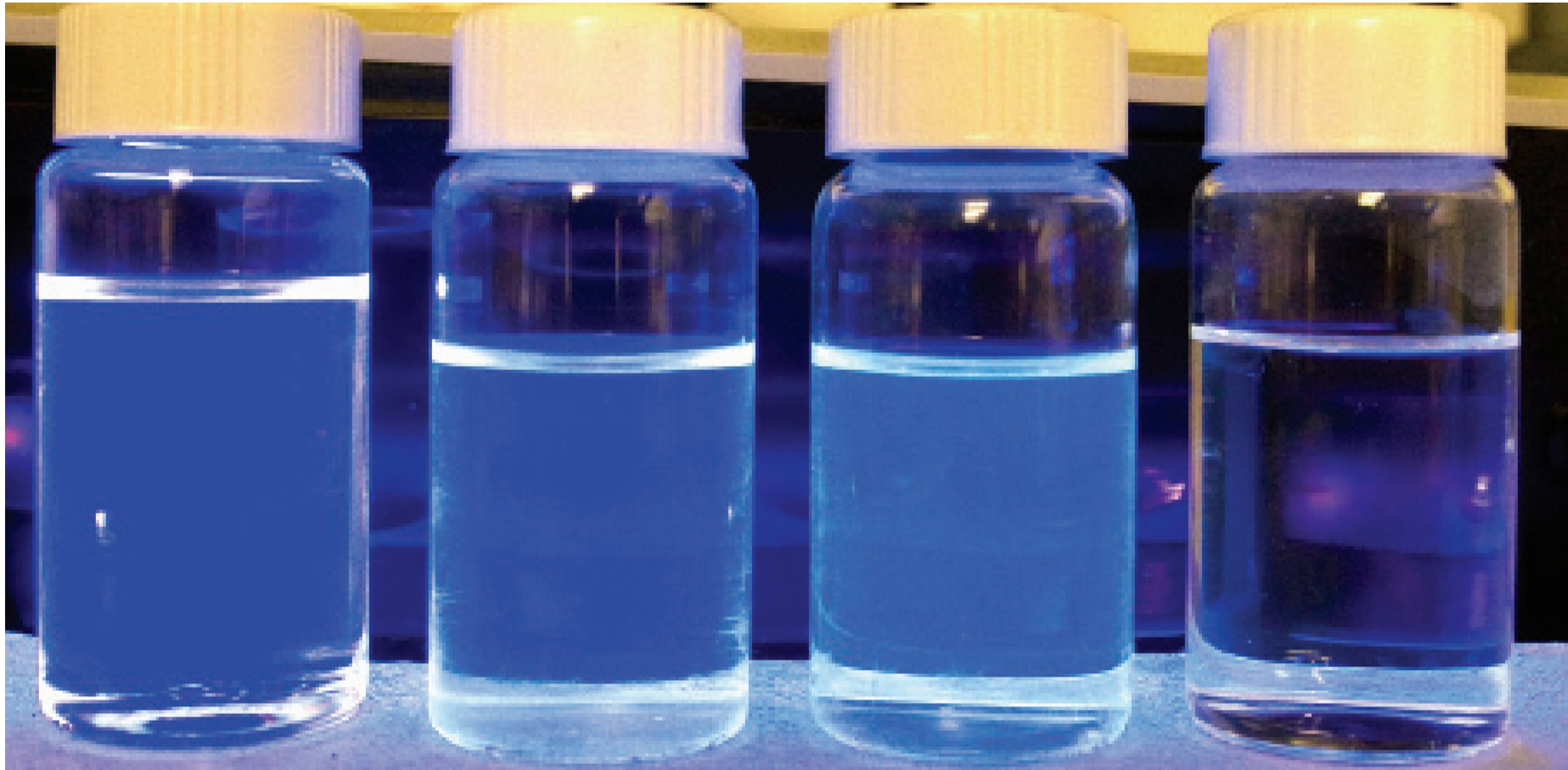


# Water-based liquid scintillator: A new detection medium



David E. Jaffe\*, BNL, 20151006

\*Cohort: **L.J.Bignell**, M.V.Diwan, S.Hans, *L.Capelluto*, S.Kettell, R.Rosero, B.Viren, E.Worcester, M.Yeh, C.Zhang [D.Beznosko, H.Themann]

# What I'm going to talk about

1. Why Water-based Liquid Scintillator (WbLS)?
  1. Successful applications of liquid scintillator(LS) and water Cerenkov detectors
  2. Possible applications of WbLS
2. WbLS properties of interest
3. Measurements
  1. Results
  2. In-progress
4. Summary and prospects



# Reactor Neutrinos - A Tool for Discoveries

*A flavor pure source of  $\bar{\nu}_e$*

2012 - Measurement of  $\theta_{13}$   
with Reactor Neutrinos

2008 - Precision measurement of  
 $\Delta m_{12}^2$ . Evidence for oscillation

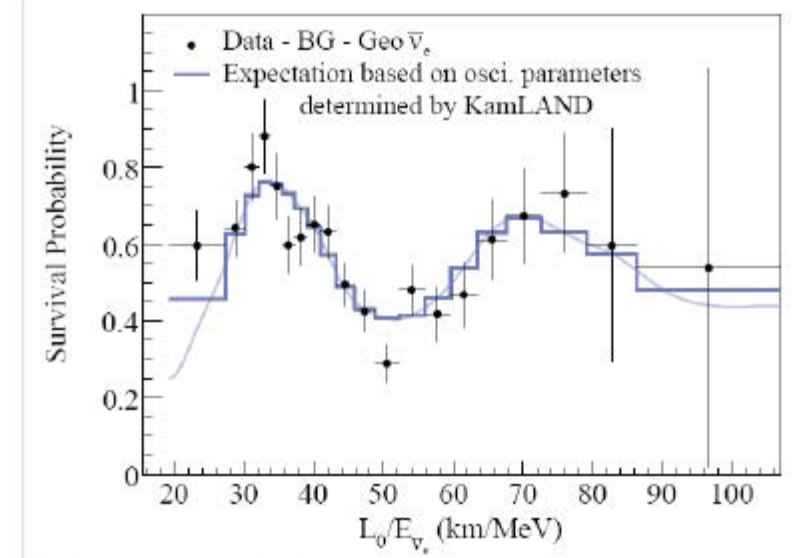
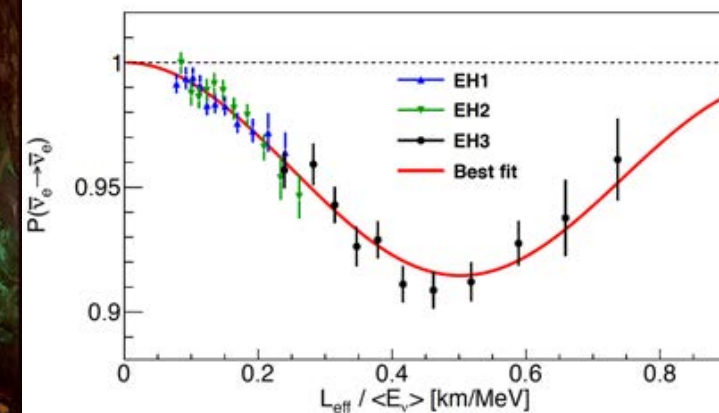
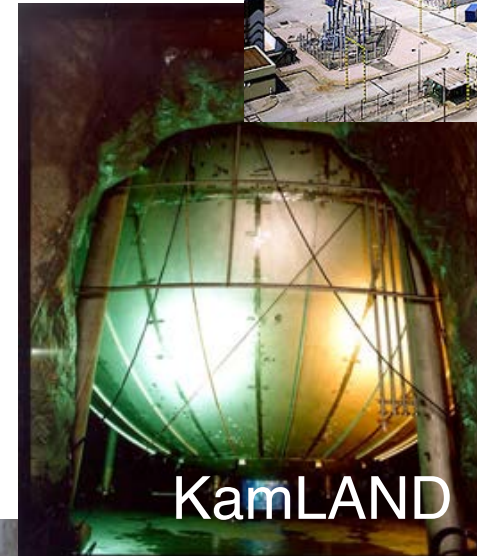
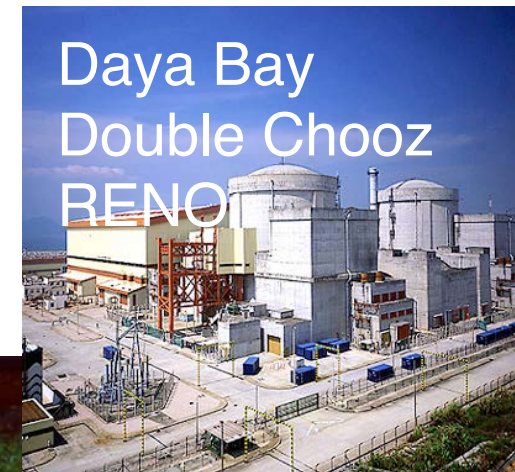
2003 - First observation of reactor  
antineutrino disappearance



1995 - Nobel Prize to Fred  
Reines at UC Irvine

1980s & 1990s - Reactor neutrino flux  
measurements in U.S. and Europe

1956 - First observation  
of (anti)neutrinos



>55 years of liquid scintillator detectors  
a story of varying baselines...

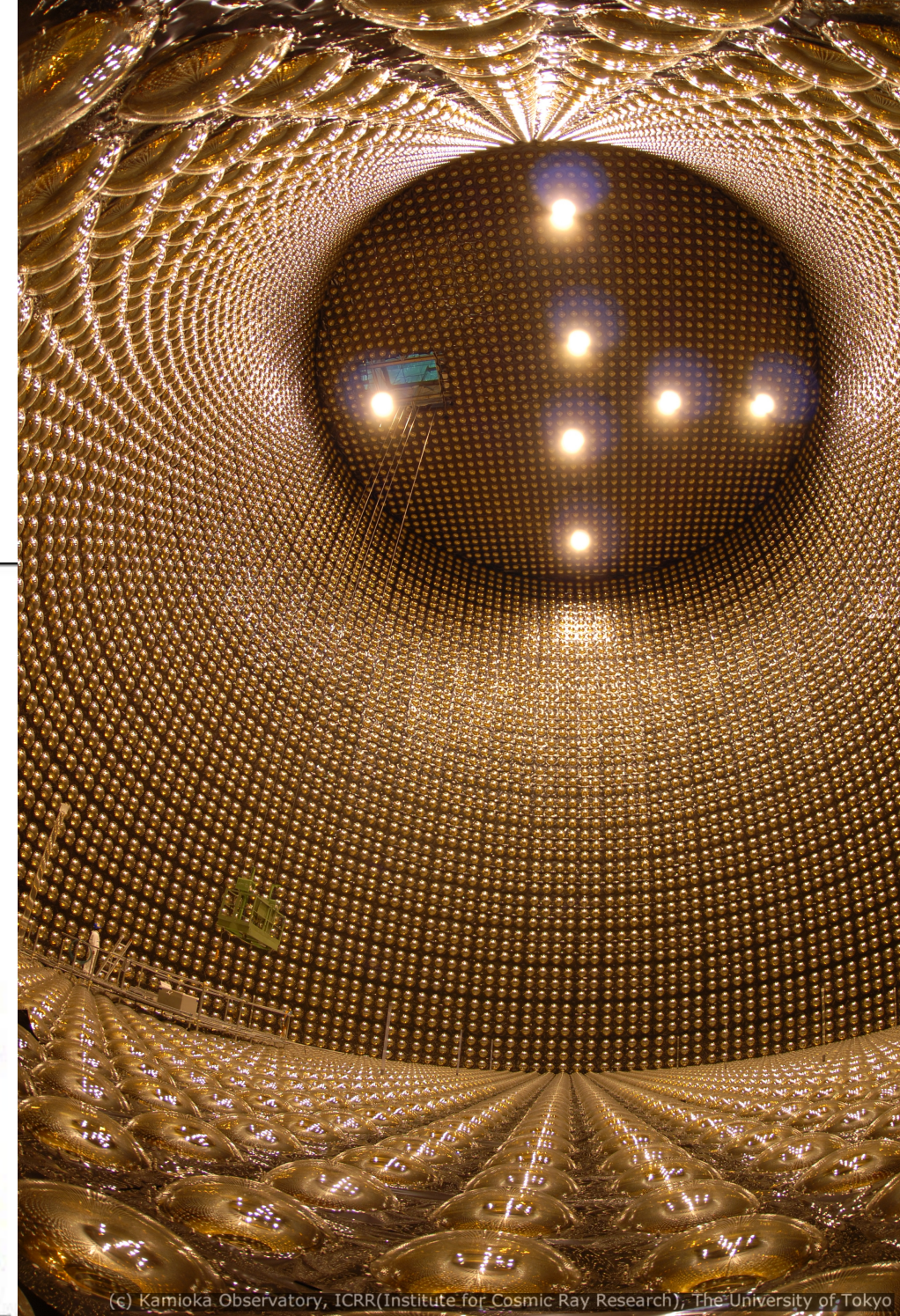
Savannah River

Karsten Heeger, Reactor Working Group Summary, WINP, 6Feb 2015 <sup>3</sup>



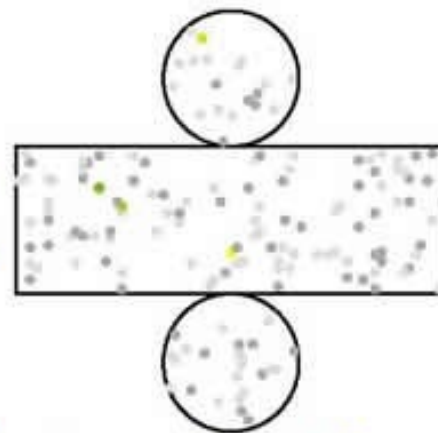
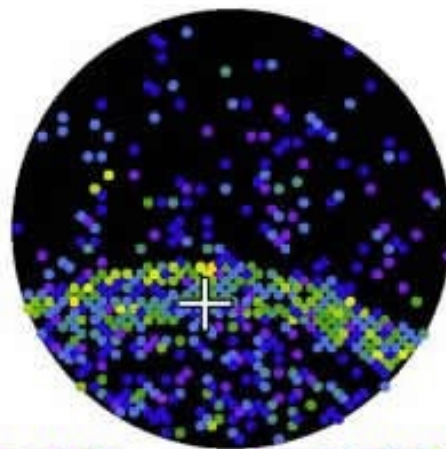
# Super-Kamiokande

Stainless steel cylinder (diameter 39m, height 42m) filled with ~50 kilotons of ultrapure water instrumented with ~11k 20" PMTs for ~40% photocathode coverage



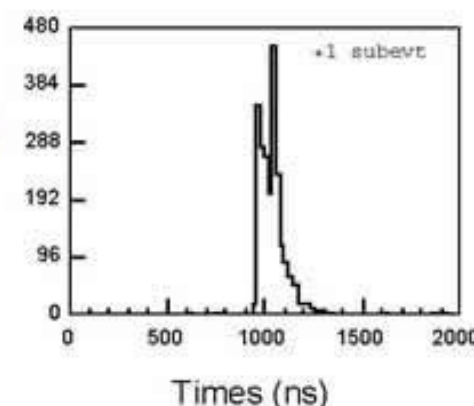
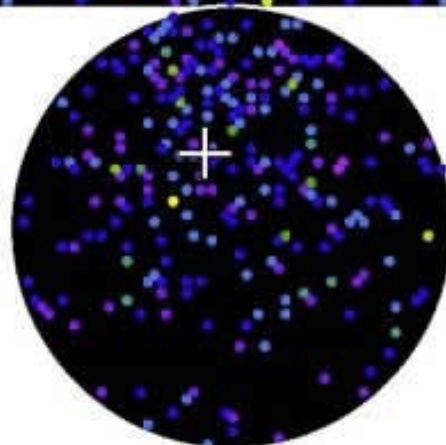
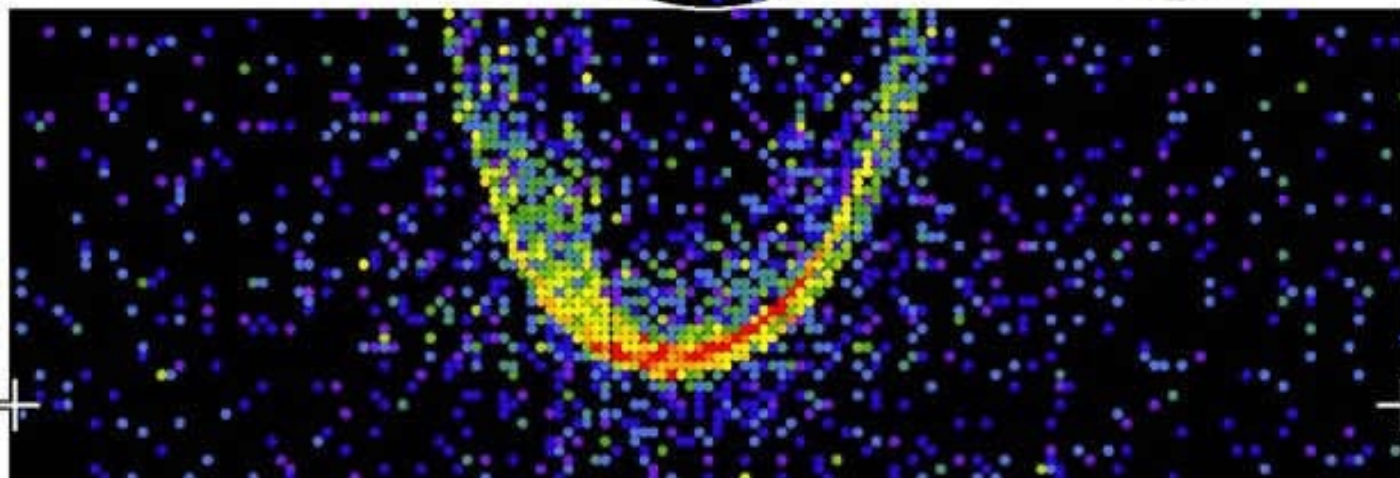
## Super-Kamiokande I

Run 1728 Sub 4 Ev 25171  
96-05-29:08:01:53  
Inner: 2294 hits, 7095 pE  
Outer: 4 hits, 32 pE (in-time)  
Trigger ID: 0x03  
D wall: 592.8 cm  
PC mu-like,  $p = 1012.9 \text{ MeV/c}$



## Charge (pe)

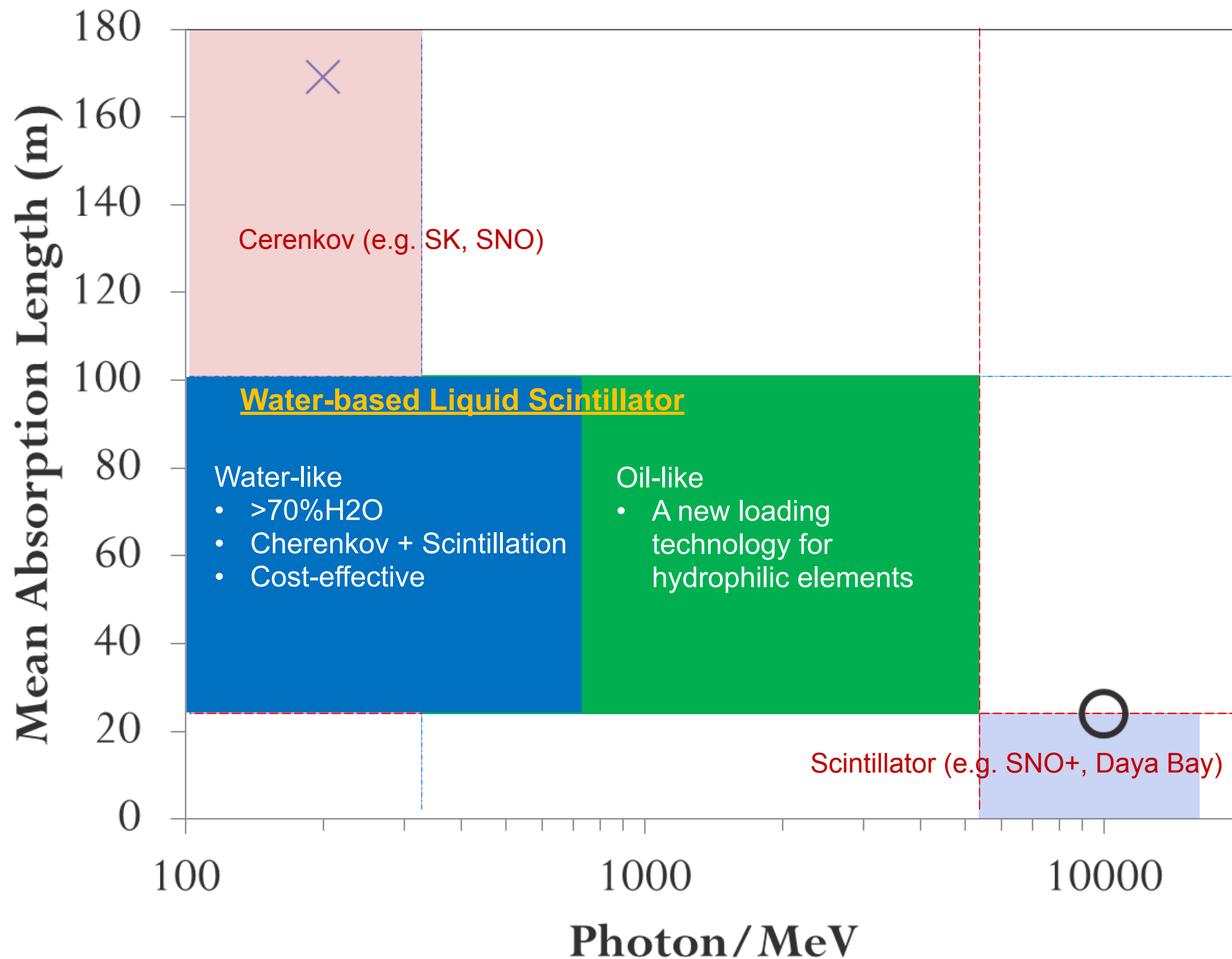
• >26.7  
• 23.3-26.7  
• 20.2-23.3  
• 17.3-20.2  
• 14.7-17.3  
• 12.3-14.7  
• 10.0-12.3  
• 8.0-10.0  
• 6.2-8.0  
• 4.7-6.2  
• 3.3-4.7  
• 2.2-3.3  
• 1.3-2.2  
• 0.7-1.3  
• 0.2-0.7  
• < 0.2



Nucl. Instrum. Methods Phys. Res.,  
Sect. A **501**, 418 (2003).



# WbLS conceptually: Absorption length vs light yield





# WbLS properties

WbLS is an emulsion and was developed by Minfang Yeh of the Neutrino and Nuclear Chemistry Group in the BNL Chemistry Department

1. Adjustable scintillation light yield ( $\sim 0.5$  to  $\sim 15\%$  LS added to water)
2. Long attenuation length (LS  $\sim 20\text{m}$ , water  $\sim 100\text{m}$ )
3. Particle identification/reconstruction:
  1. Directional (Cerenkov) and isotropic (Scintillation) light
  2. Timing of prompt Cerenkov and scintillation light
  3. Energy measurement via calorimetry (scint.) and Cerenkov threshold
4. Low-cost: Primary material is pure water
5. Environmentally and chemically friendly
6. Enables dissolution of lipophobic but hydrophilic metals



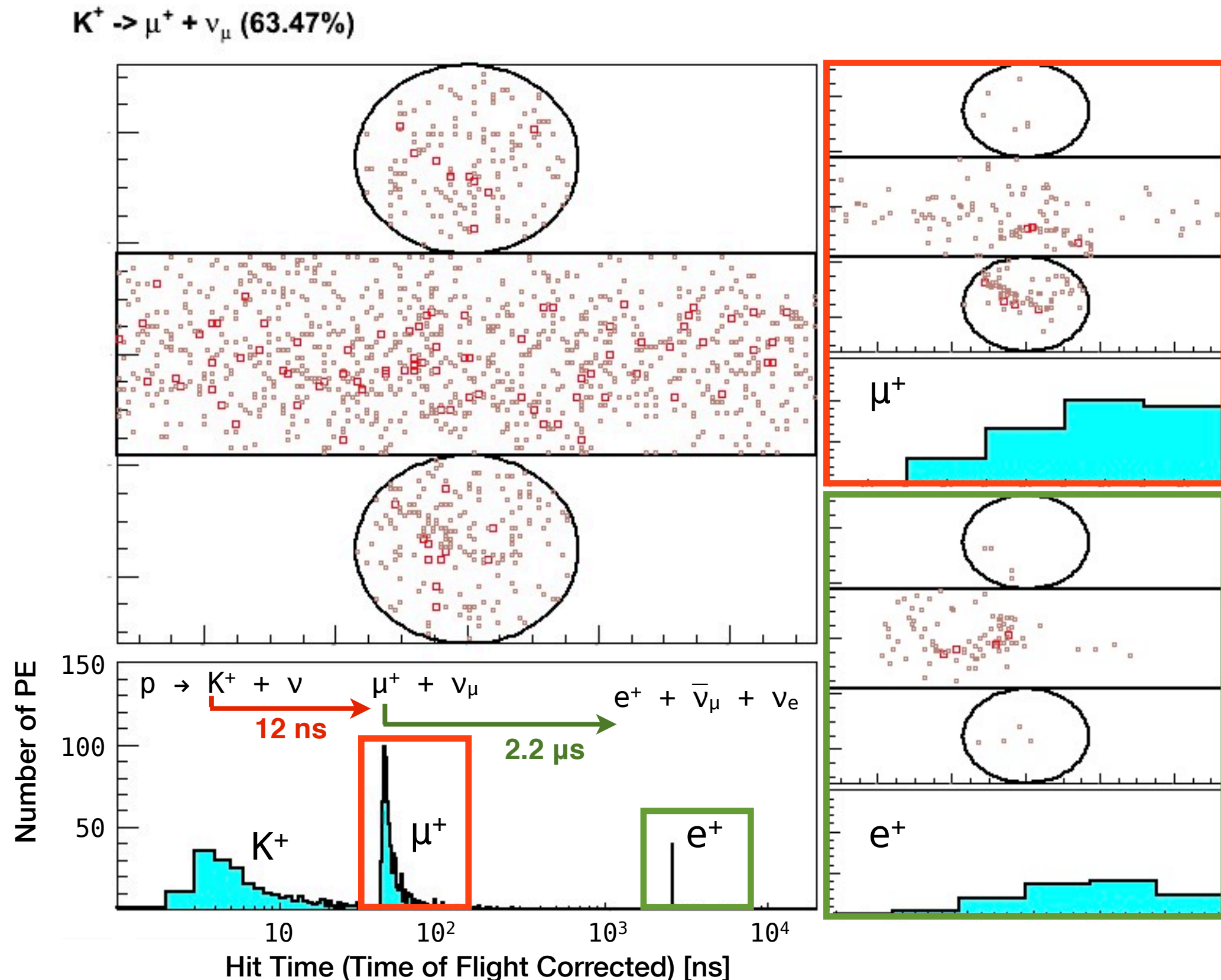
# Some applications

1.  $p \rightarrow K^+ \nu$  : Favored by a number SUSY GUTs,  $K^+$  is below Cerenkov threshold in water, WbLS makes  $K^+$  detectable
2. Neutrino-less double-beta decay ( $0\nu\beta\beta$ ): Are neutrinos Dirac or Majorana particles? WbLS + improved photodetector may be a way to access isotopes at the  $\sim 50$ ton-scale
3. Beam therapy quality assurance: Real-time hadron therapy dose verification in water-equivalent phantom

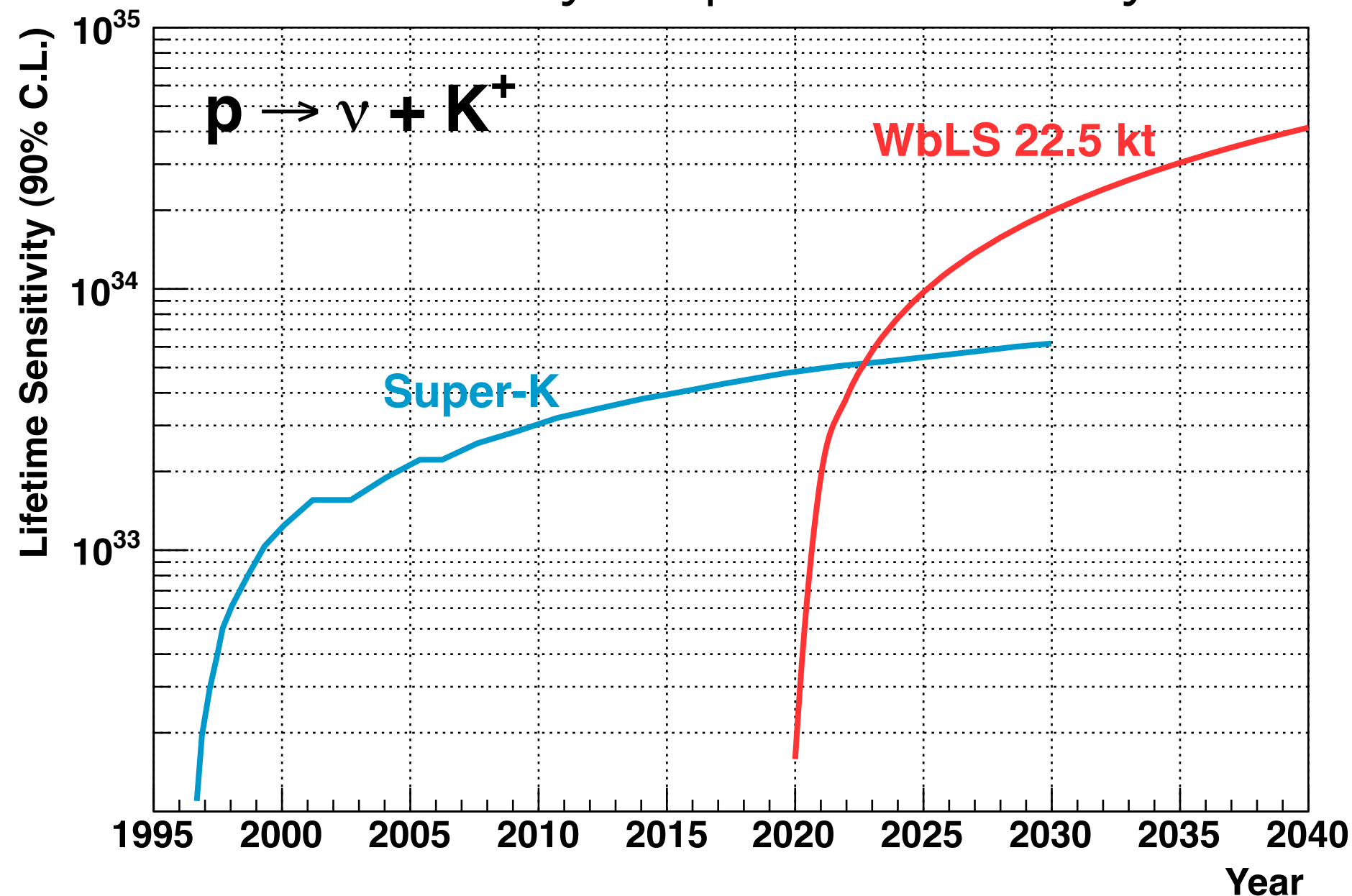


# Increased sensitivity to proton decay with WbLS

Simulated event with 90 optical photons/MeV (**~1% WbLS**) in a SuperKamiokande-sized detector. Note: WLS of Cerenkov photons not taken into account in this simulation.



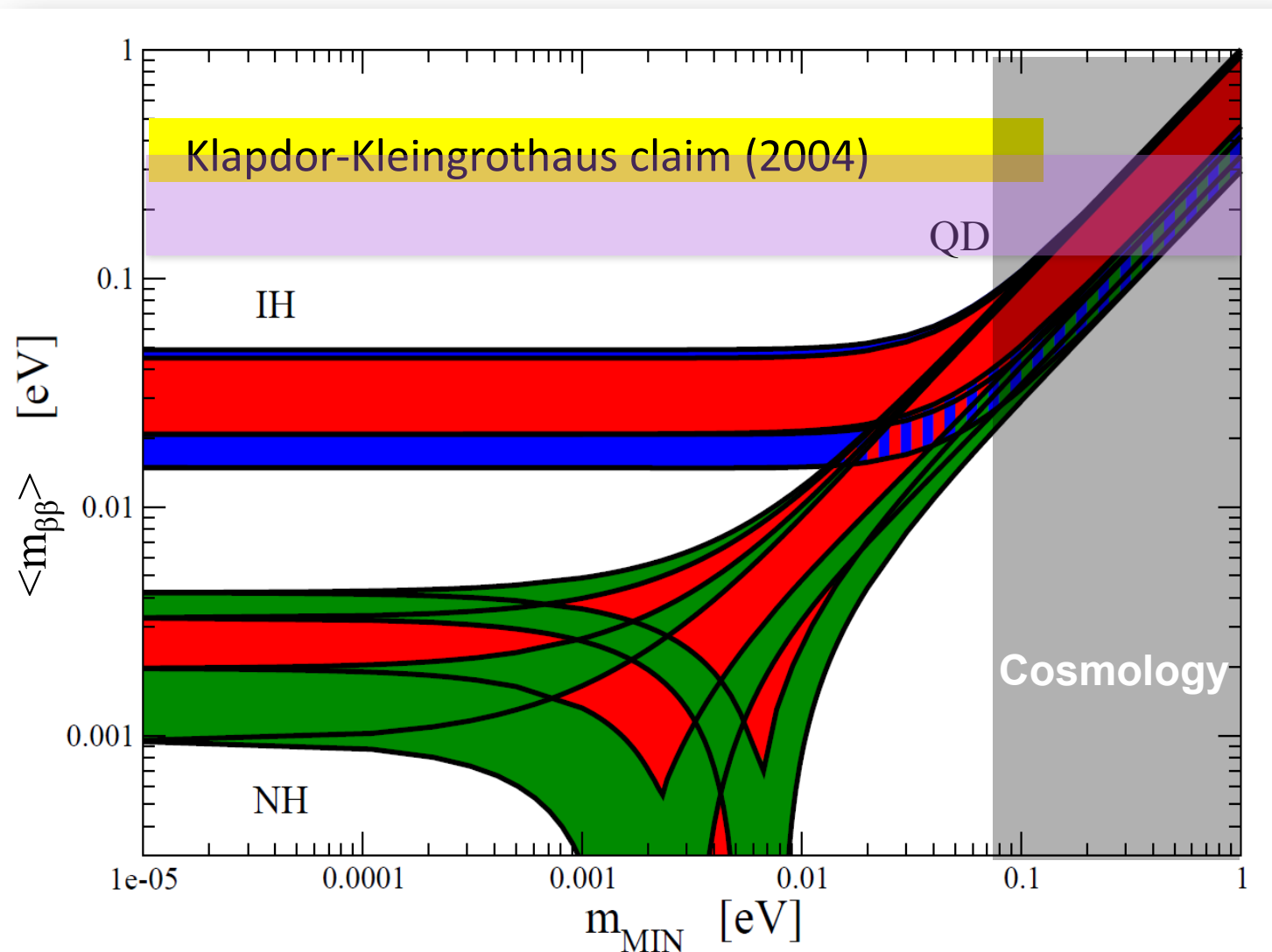
# Increased sensitivity to proton decay with WbLS



1. Main background is due to atmospheric muon neutrinos
2. Estimated signal efficiency of 88% based on selection on time, charge and particle ID with a background rejection of >99.975%
3. Expected 0.1 background per 10 years



# Kinematically allowed Neutrino-less double-beta decay ( $0\nu\beta\beta$ ) regions given knowledge of neutrinos



90%CL upper limit  
 $\langle m_{\beta\beta} \rangle < 129-341 \text{ meV}$   
 $T_{1/2} > 1.9 \times 10^{25} \text{ yr}$   
 Exposure 85 kg.yr  
 P.Decowski, TAUP2013

Note: colored bands  
 Indicate allowed  
 variation of  $U_{ei}$  due to  
 unknown Majorana  
 phases and uncertainty  
 in mixing angles

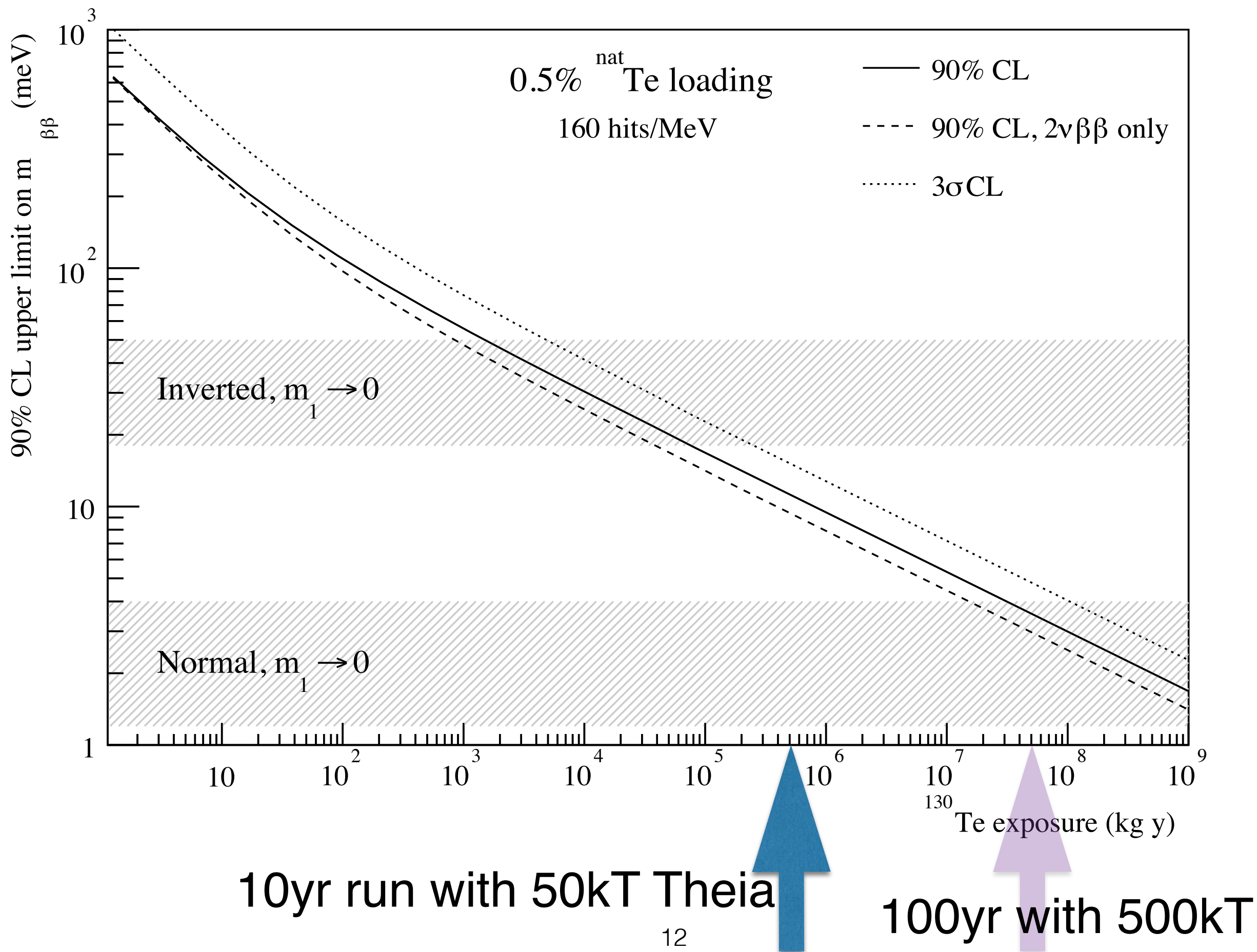
- $\langle m_{\beta\beta} \rangle^2 = \left| \sum_i U_{ei}^2 m_{\nu_i} \right|^2$
- $m_{\text{MIN}} = \text{lightest } m_{\nu_i}$

R.D.McKeown, Report to Nuclear Science Advisory Committee, Neutrinoless Double Beta Decay, April 2014

# $0\nu\beta\beta$ with WbLS-based detector

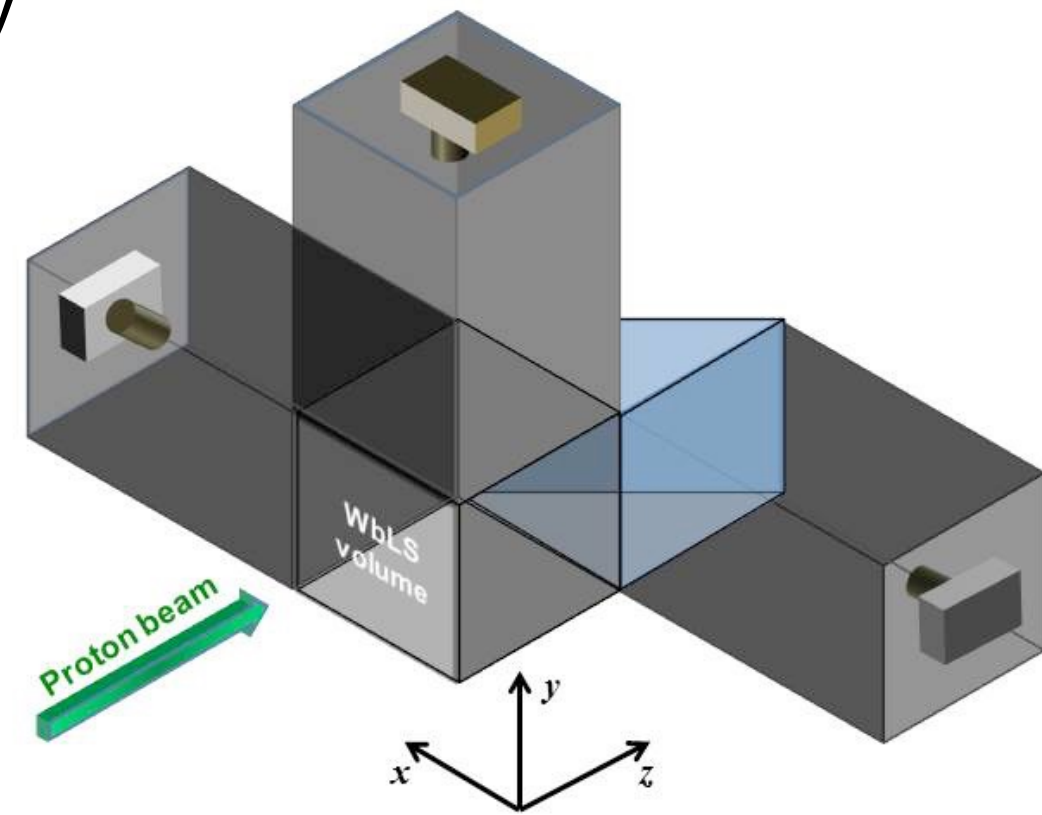
1. SuperK-size (50kT) detector with **4%WbLS**. Need 5.5% energy resolution at  $\beta\beta$  endpoint ( $\sim 160$  pe/MeV).
2. Nearly 100% photocathode coverage of high quantum efficiency photodetectors, eg. Hamamatsu R11780 or Large Area Picosecond PhotoDetector (LAPPD)
3. 0.5% loading of  $^{\text{nat}}\text{Te}$  in WbLS would have  $\sim 50\text{T}$   $^{130}\text{Te}$  (34% abundance). Same  $0\nu\beta\beta$  isotope as proposed for SNO+
4. Concept elaborated and discussed in <http://arxiv.org/abs/1409.5864>, “Advanced Scintillator Detector Concept (ASDC)...”. Rich physics program including proton decay, solar neutrinos ( $^7\text{Li}$  loading of WbLS), geo-neutrinos, supernova neutrinos, diffuse supernova background neutrinos, long baseline neutrino physics (in conjunction with accelerator neutrino source), sterile neutrinos (in conjunction with neutrino source). ASDC also known as “Theia”.





# Medical application of WbLS

1. Intensity-modulated pencil proton beam therapy (IMPT) in which a tumor can be targeted for radiation while sparing the surrounding healthy tissue.
2. Uses the Bragg peak of stopping protons to localize dose
3. WbLS-based “phantom” would serve as a real-time quality assurance device\*
4. Requirements on WbLS:
  1. Able to withstand  $\sim 600\text{Gy}$  yearly facility dose
  2. Understanding of light yield and collection to  $\sim 1\text{-}2\%$ .
  3. Millimeter scale position resolution
  4.  $\sim 5\%$  concentration of LS in water (“5%WbLS”)



\*Humans are “ugly bags of mostly water” - Star Trek Next Generation.



WbLS properties of interest

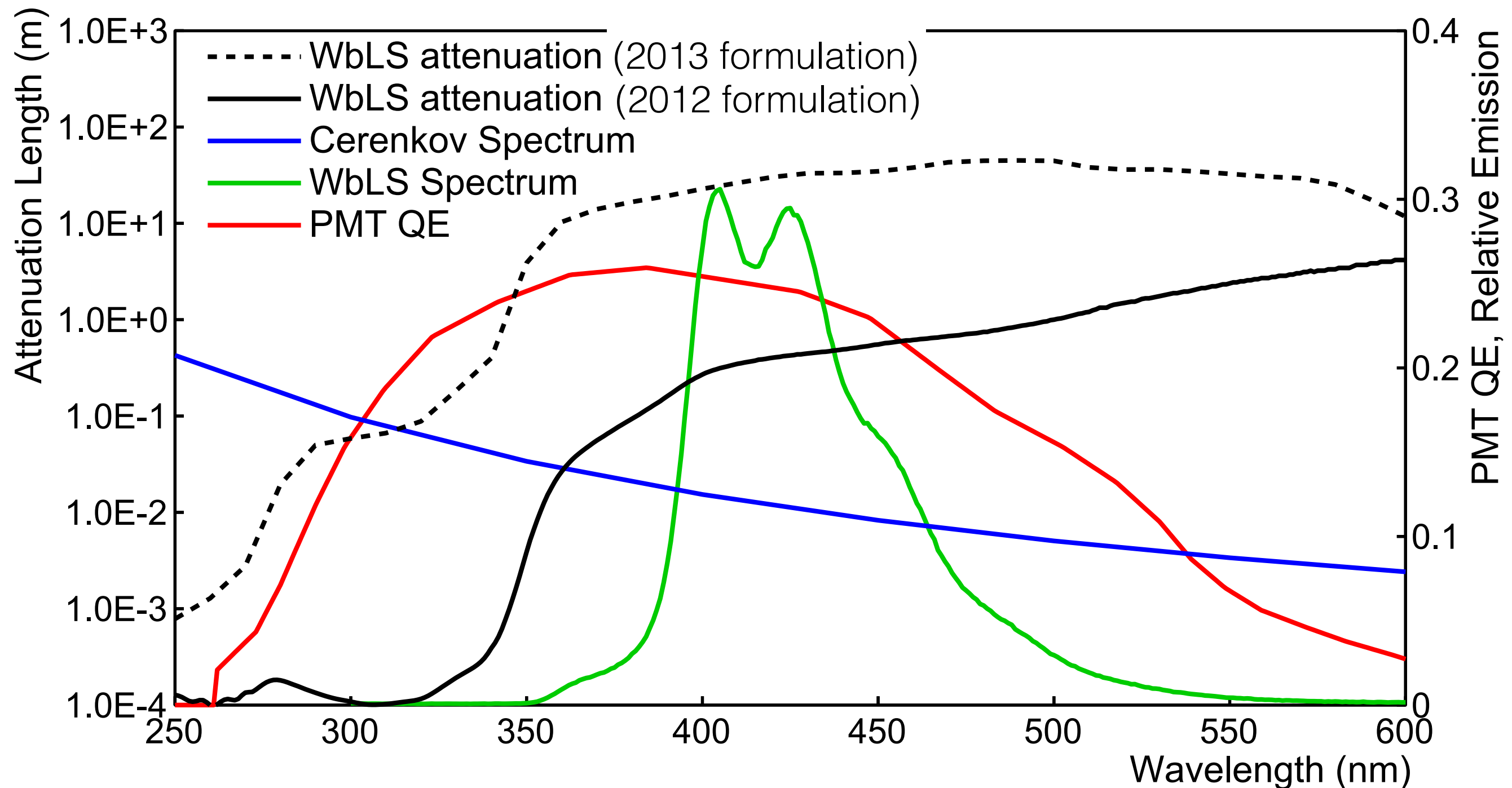
# Light production & transport in water, LS and WbLS

1. Cerenkov (point source, directional, prompt)
  1. Light yield is calculable:  $N = (\text{path length}) \times N_0(\sin^2 \Theta_C)$
  2. Spectrum  $LY(\lambda) \propto 1/\lambda^2(1-\beta^2 n(\lambda)^2)$
2. Scintillation (point source, isotropic, extended in time)
  1. Light yield proportional to energy deposit, modulo quenching. Must be measured.
  2. Narrow spectrum
3. Absorption & re-emission (possibly diffuse source, isotropic, extended in time)
  1. Optical photons from Cerenkov or scintillation process can be absorbed and re-emitted by medium
  2. Has potential to shift Cerenkov photons from UV to visible for a typical photodetector (eg. bialkalai PMT)

Light yield for these processes is comparable for <10% concentration WbLS. Disentangling them and understanding the details of wavelength-dependence is the main focus of R&D.



# Wavelength-dependence of attenuation, emission, PMT quantum efficiency



Light yield for these processes is comparable for  $<10\%$  concentration WbLS. Disentangling them and understanding the details of wavelength-dependence is the main focus of R&D.

# Characterizing WbLS

1. Light yield (photons/MeV)
2. Absorption & emission spectra
3. Quantum yield (#photons emitted/# photons absorbed)
4. Quenching
5. Pulse shape discrimination
6. Fluorescence & scintillation decay time
7. Attenuation length
8. Colloid size
9. Colloid electrokinetic or “zeta” potential
10. Stability
11. Compatibility
12. Radiation hardness
13. Metal-loading capability

# Measurements

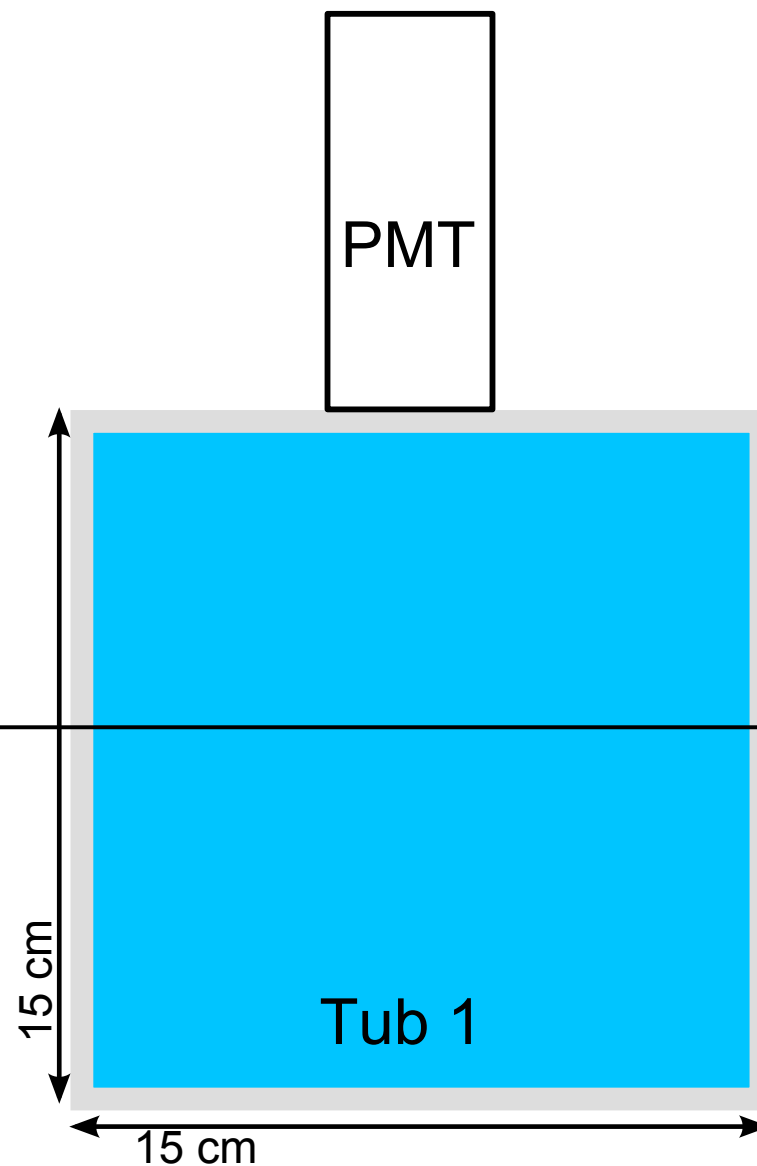


1. Samples investigated (“2012 WbLS” formulation)
  1. Pure water.
  2. 0.4% WbLS = “WbLS-1”  
0.4%PC (pseudocumene)+0.4g/L PPO+3mg/L MSB+ surfactant + water
  3. 1% WbLS = “WbLS-2”  
1.0%PC+1.36g/L PPO+7.48mg/L MSB + surfactant + water
  4. LS: LAB(Linear Alkyl Benzene) + 2g/L PPO + 15mg/L MSB.
2. Low energy proton beam data at NSRL (NASA Space Radiation Laboratory at BNL)
  1. *NSRL run 12C*: Measure light yield for 4 samples & investigate quenching with 2000 MeV (~minimum ionizing), 475 MeV (Cerenkov threshold in water), 210 MeV ( $\beta p = \beta_K$  for  $p \rightarrow K^+ \nu$ )
  2. *NSRL run 13A*: Calibrate 1% WbLS light yield against Cerenkov light yield, disentangle competing light production processes with 2000 & 475 MeV beams
3. Fluorescence and UV-VIS spectrometry (absorption and (re-)emission)
4. Light yield from Compton-scattered electrons with a  $^{137}\text{Cs}$  gamma source

# NSRL12C apparatus: Identical liquids in T1,T2

210MeV  
475MeV  
2000MeV  
Protons  
Beam

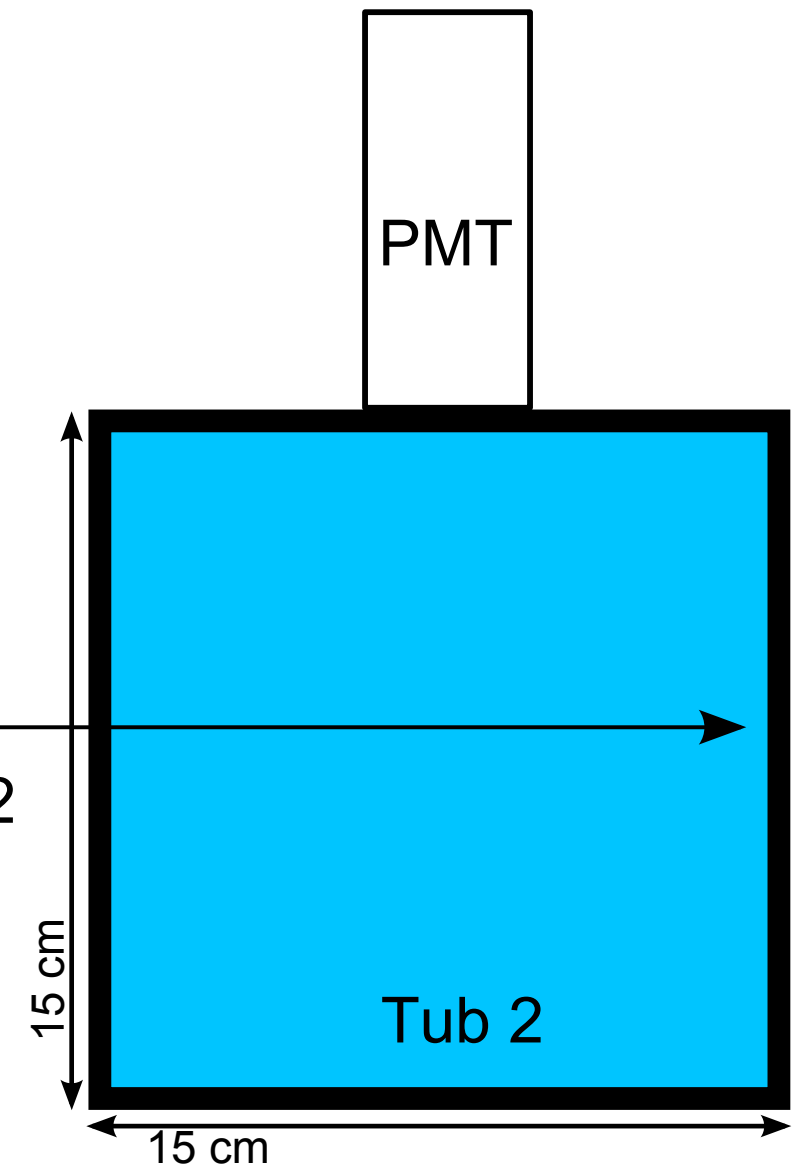
H1



Tub 1

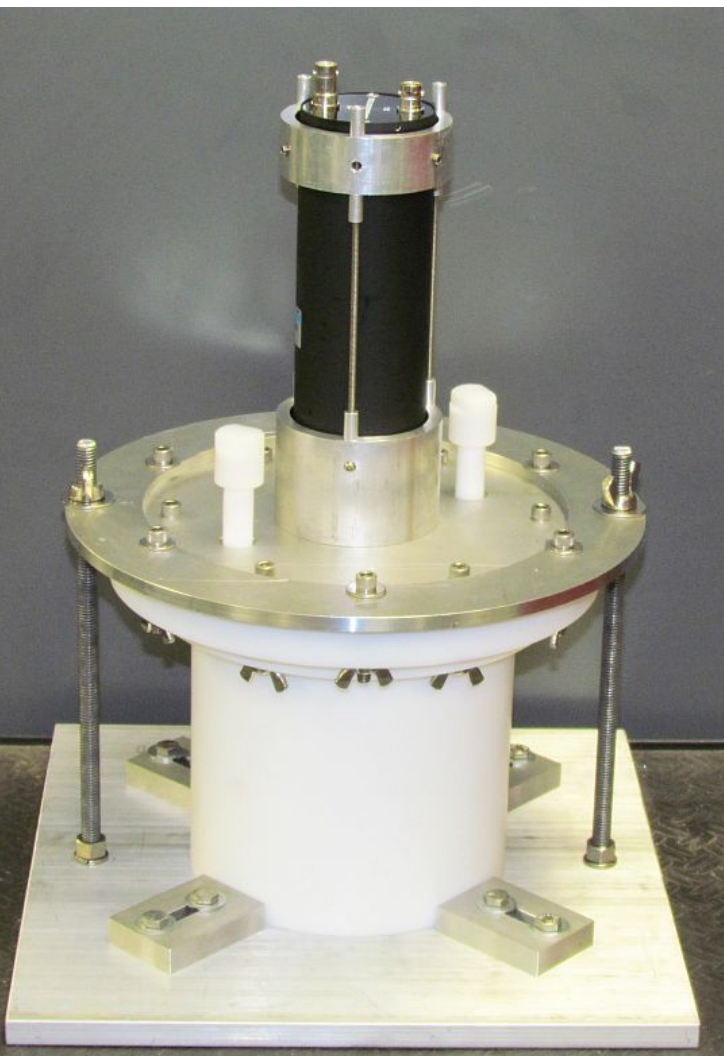
High-reflectivity  
white PTFE

H2



Tub 2

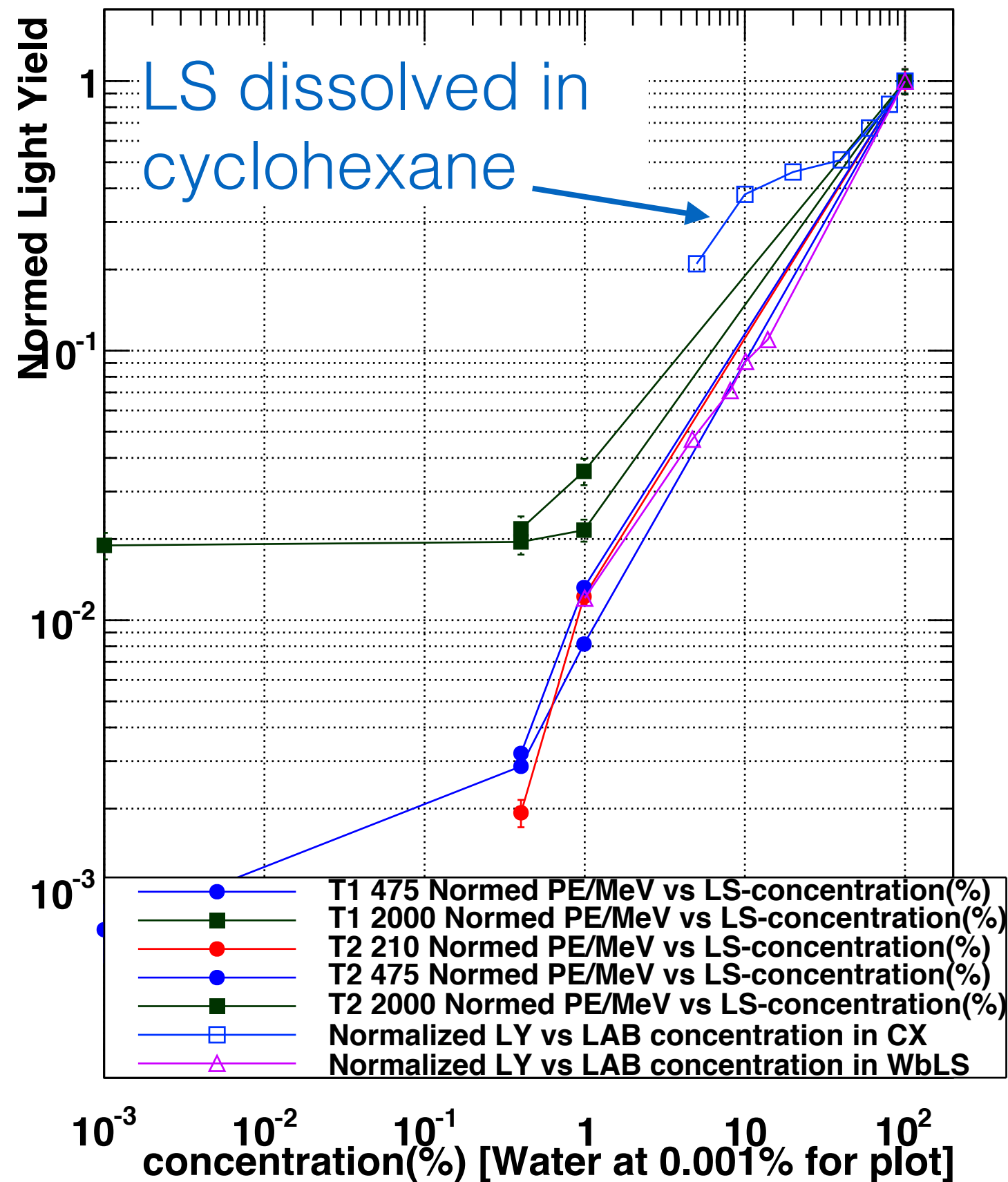
Al coated with low  
reflectivity black PFA

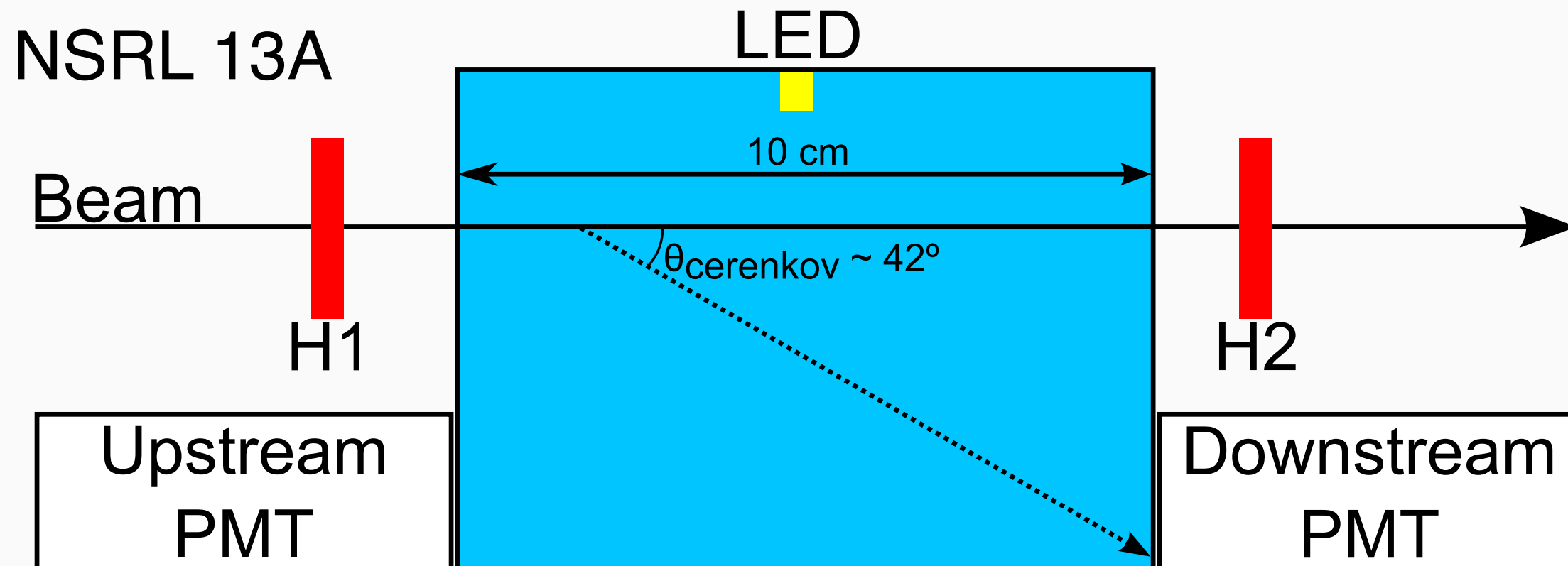


# Compare NSRL12C proton & Compton-edge data

Comparison of relative light yield of  
proton beam data with Compton-  
edge data for WbLS and **LS  
dissolved in cyclohexane(CX)**

1. Light yield roughly proportional to concentration in WbLS emulsion
2. In cyclohexane, light yield higher at low concentrations
3. Cerenkov effect apparent for 2000 MeV proton data





**Figure:** The beamline detector setup.

- Proton beam incident on 1% WbLS or water.
  - 1% WbLS: 1% Pseudocumene, 1.36 g/L PPO, 7.48 mg/L Bis-MSB, water, surfactant.
- Black ABS plastic vessel, UV-transparent acrylic windows to PMTs (Hamamatsu R7723).
- Plastic scintillator hodoscopes define 2 x 2 cm beam (H1 & H2).
- LED in target volume for in-situ single PE calibration.

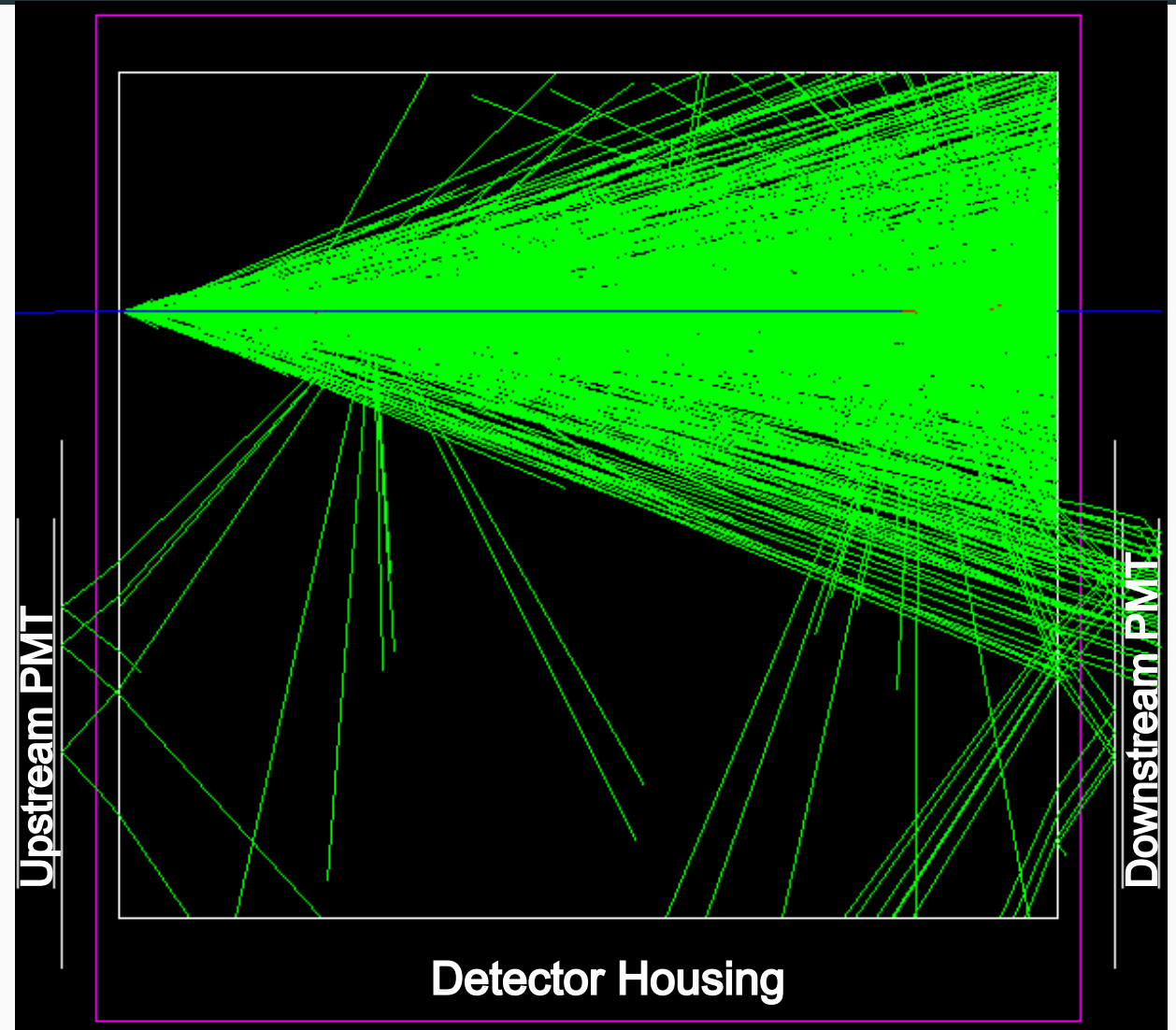


# SIMULATION MODEL DESCRIPTION

Geant4.10 simulation of the detector and hodoscopes, with customized wavelength-shifting (WLS) physics to incorporate:

- wavelength-dependent quantum yield<sup>3</sup>
- wavelength-dependent emission spectrum

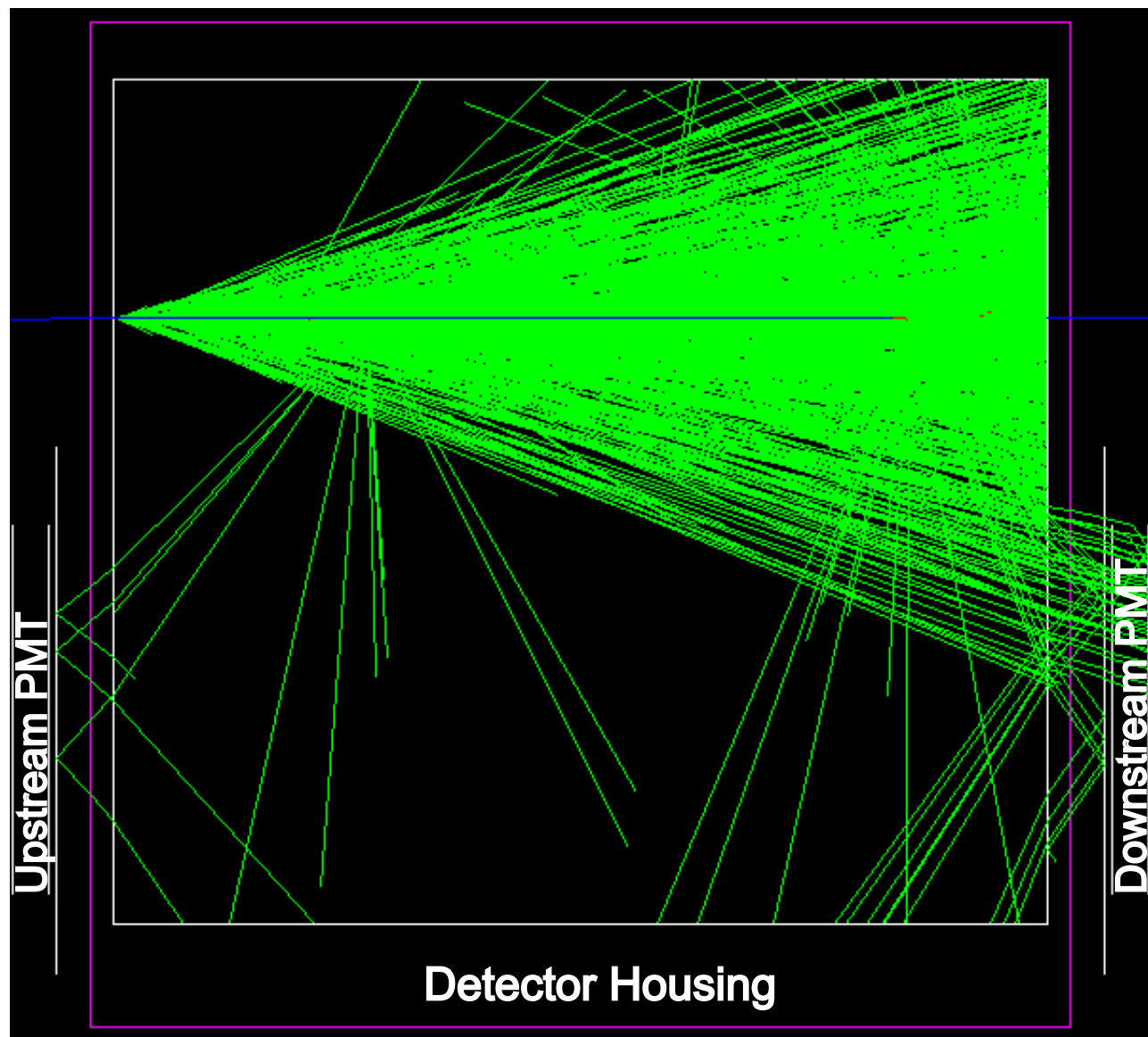
Wavelength-dependent PMT quantum efficiency implemented in readout.



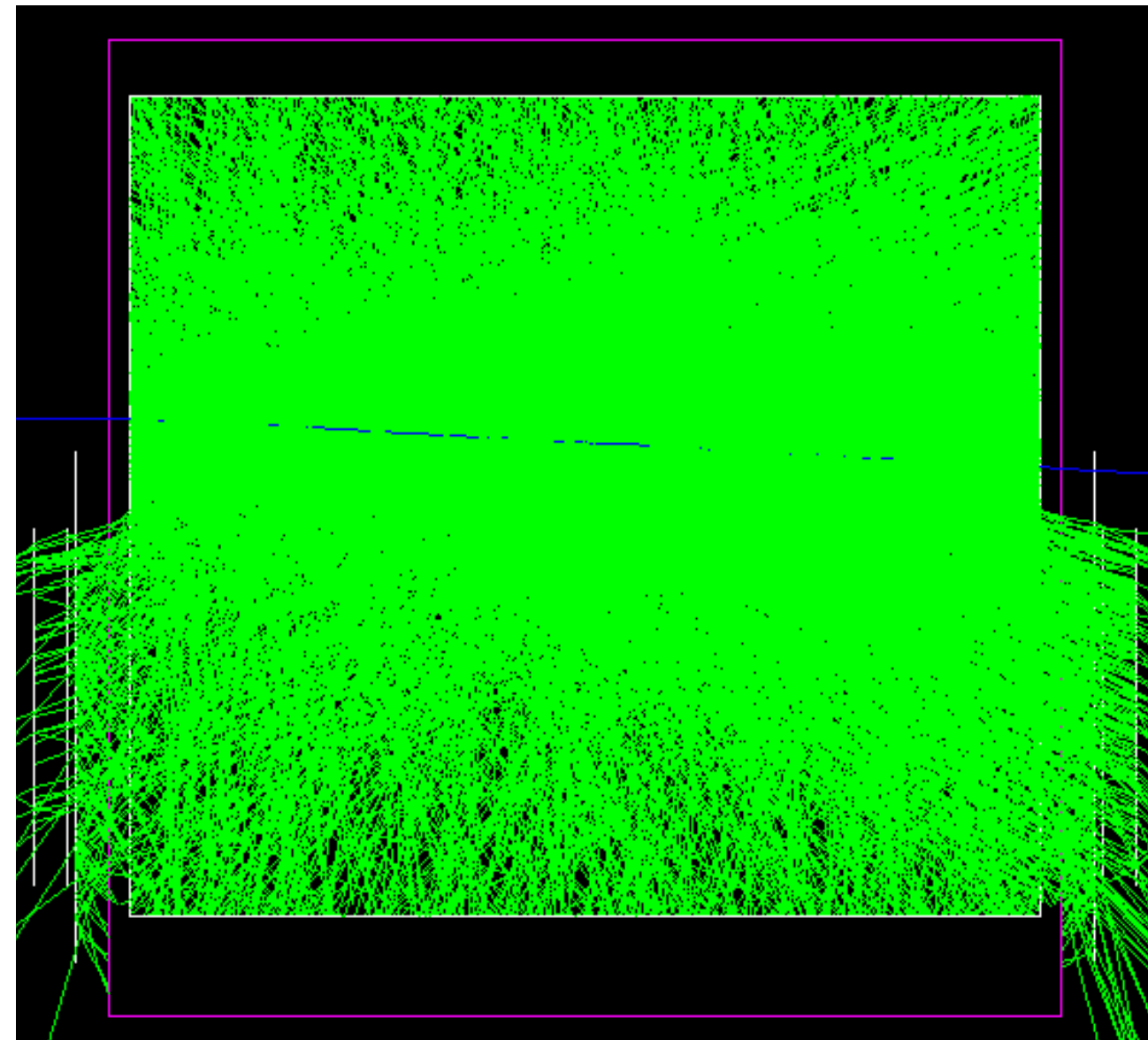
**Figure:** A simulated 2 GeV proton (blue) event in water, with Cerenkov photons (green). The Cerenkov cone illuminates the downstream PMT. Cerenkov photons produced by secondary electrons are also visible.

---

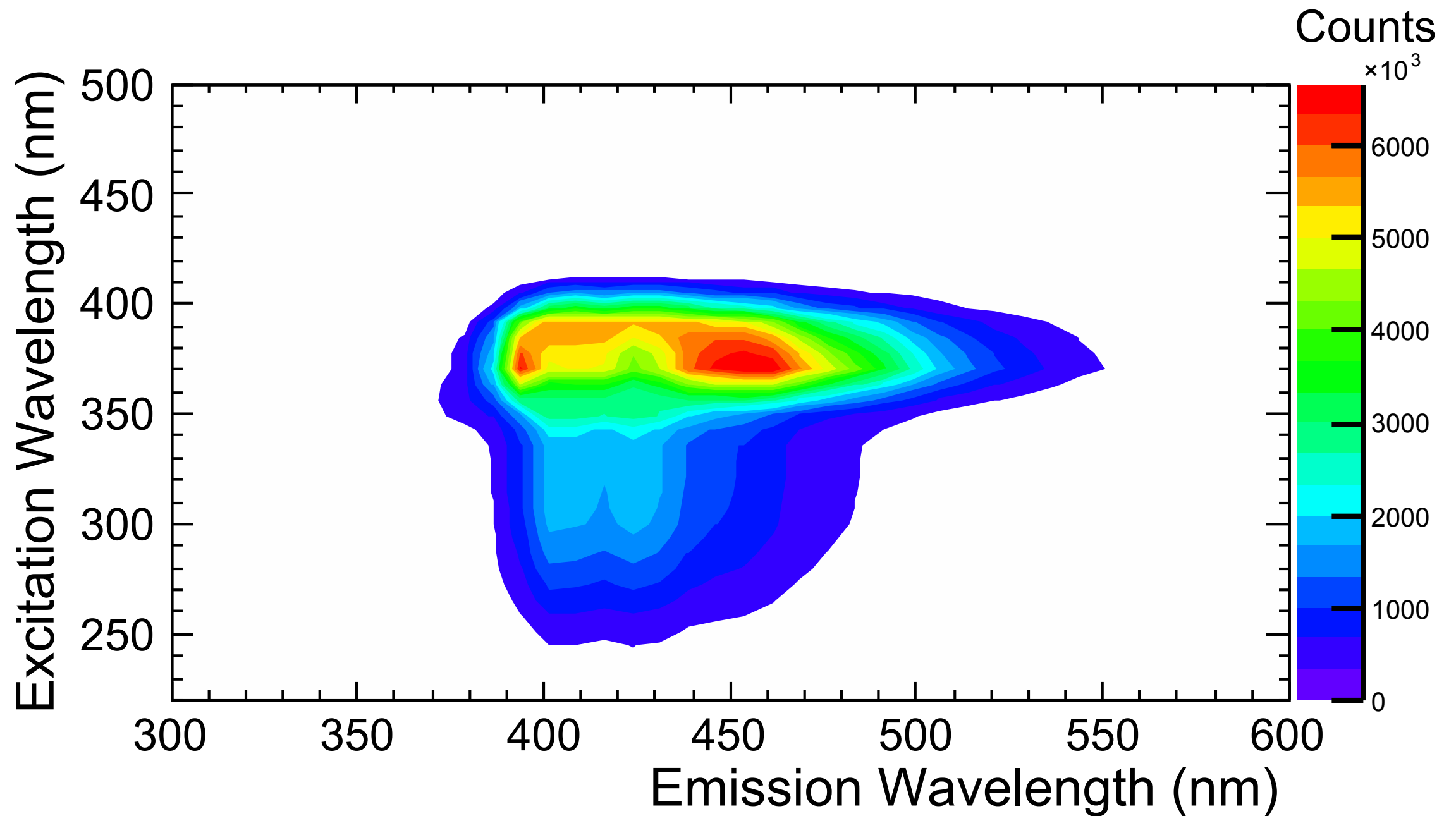
<sup>3</sup>The quantum yield of a fluorescent material is defined as the probability of emission, upon absorption of a photon.



Simulated 2000 MeV proton beam in water



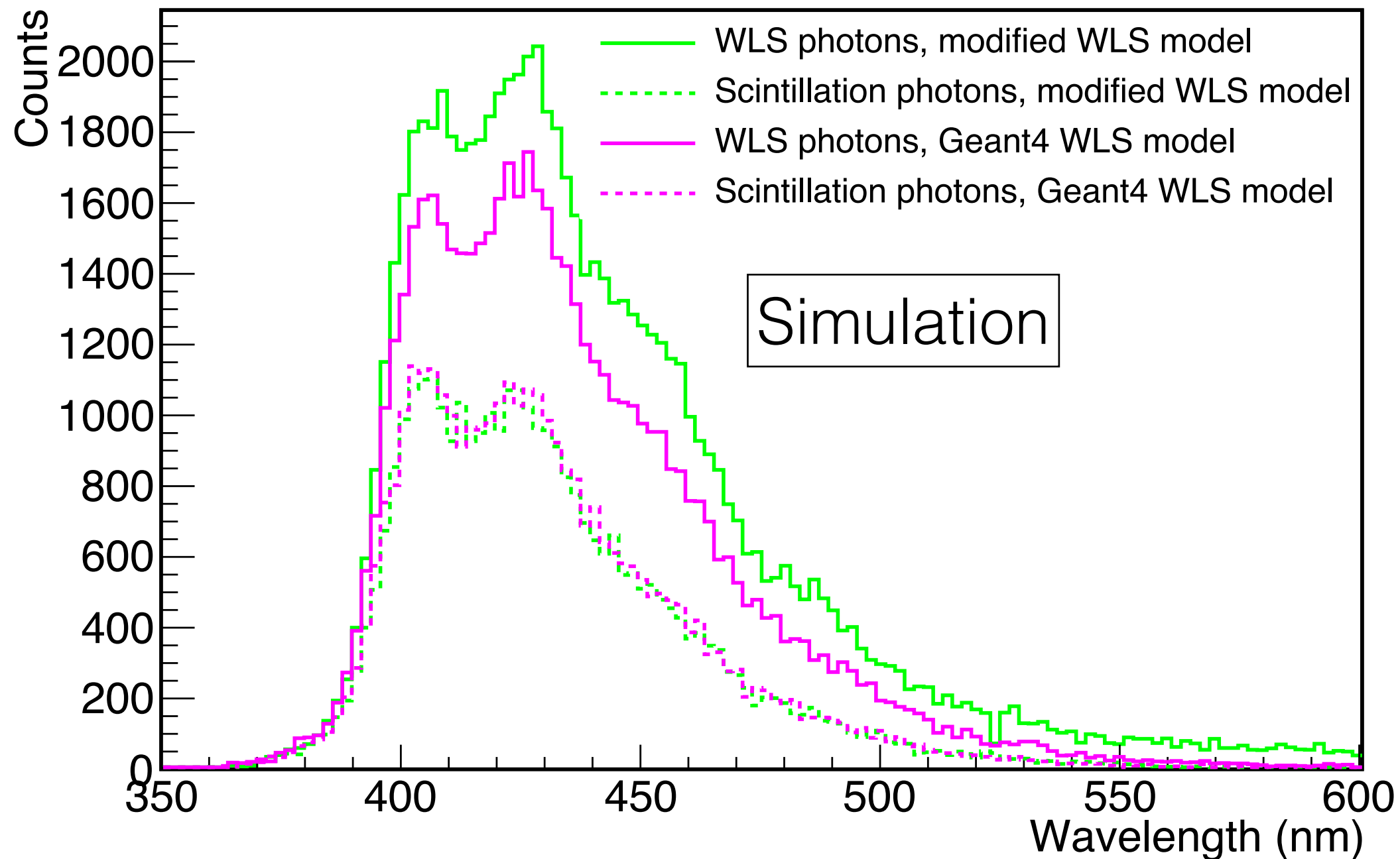
Simulated 2000 MeV proton beam in 1% WbLS



# Excitation vs Emission for 1%WbLS

Measured with PTI fluorescence spectrometer and used  
in simulation

# Predicted optical photon spectrum from WbLS for 2GeV



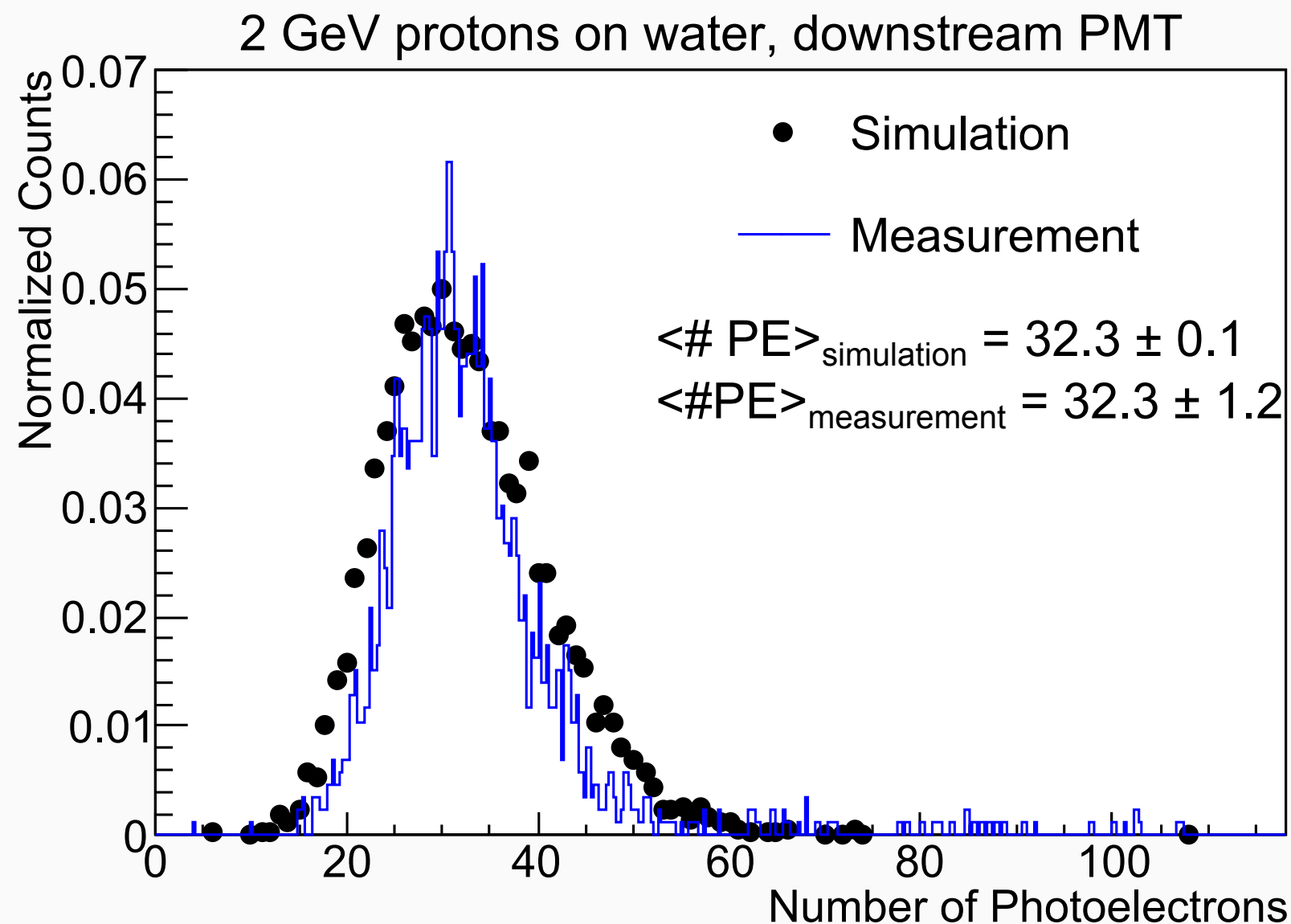
Modified WaveLength Shifting (WLS) model predicts 27% more WLS light and 20% more overall light from 1% WbLS in upstream PMT for 2 GeV protons



## 2 GEV PROTONS ON WATER – MODEL CALIBRATION

Simulated optical parameters were optimized to the water measurements.

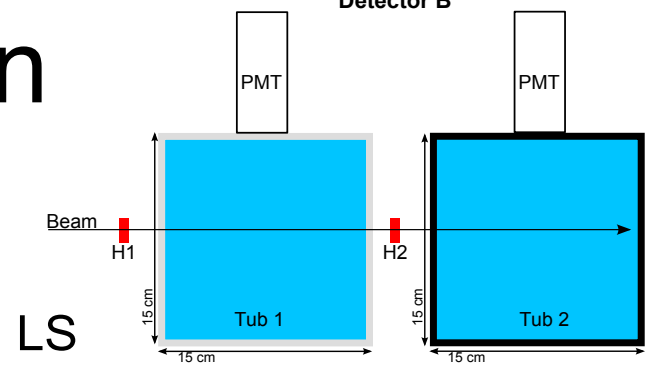
2 GeV water measurements confirmed validity of simulated geometry and readout.



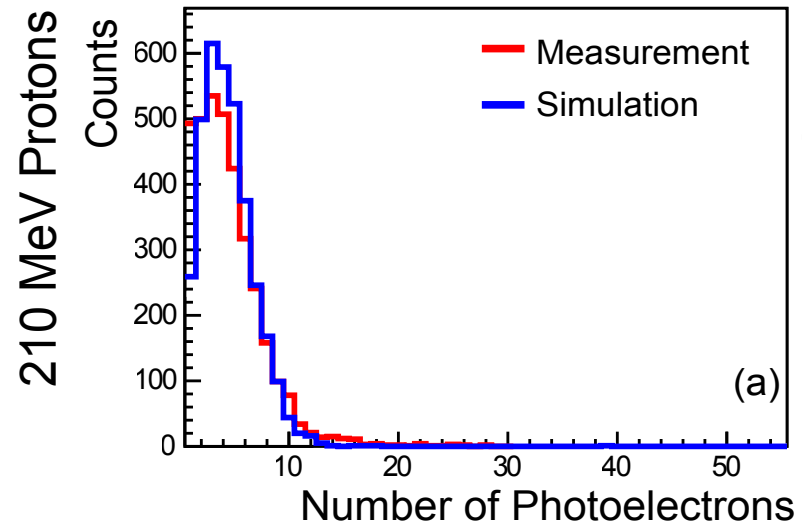
Slight difference in width of distributions not understood

# Comparison of NSRL12C data with simulation

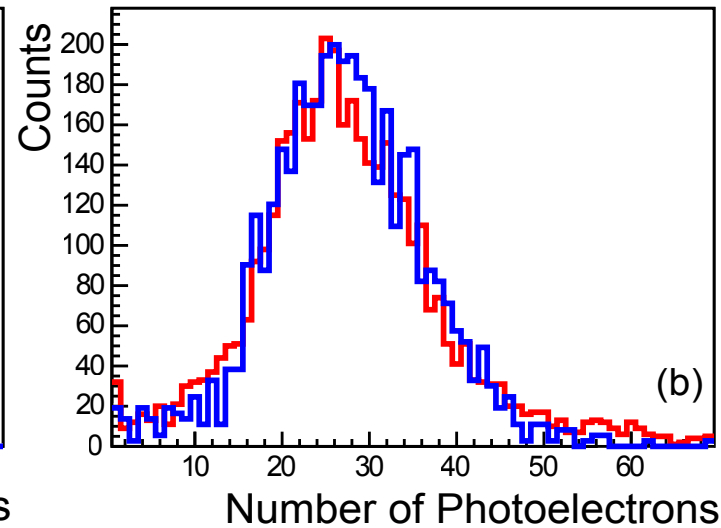
## Sample composition



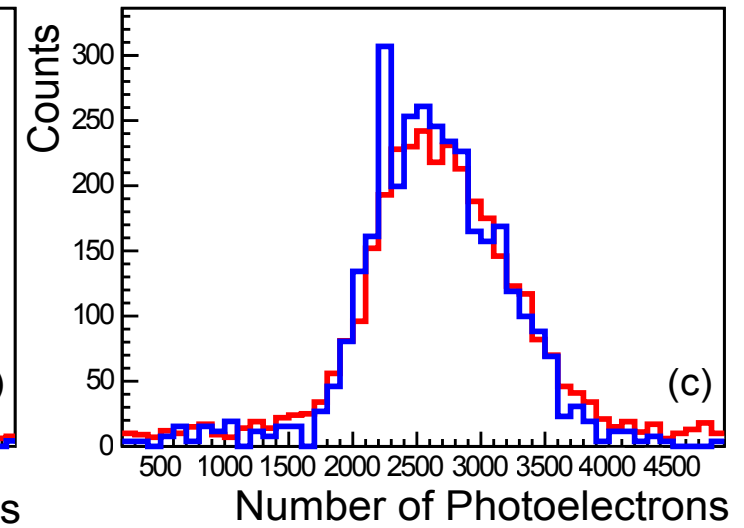
WBLS-1



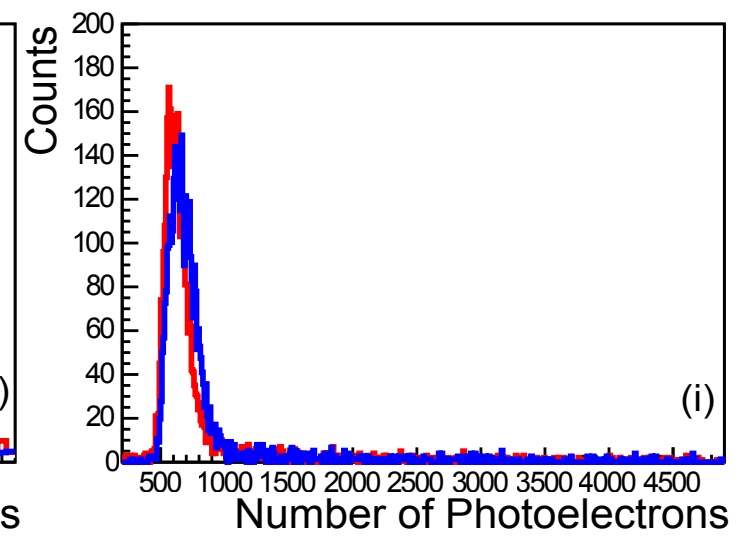
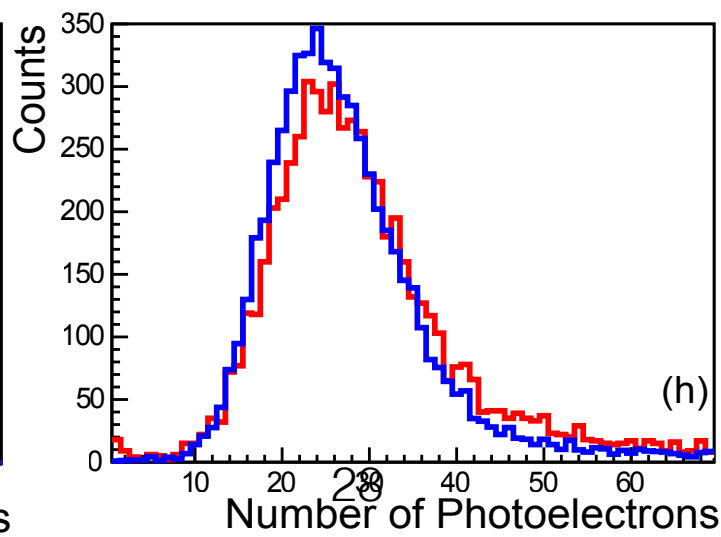
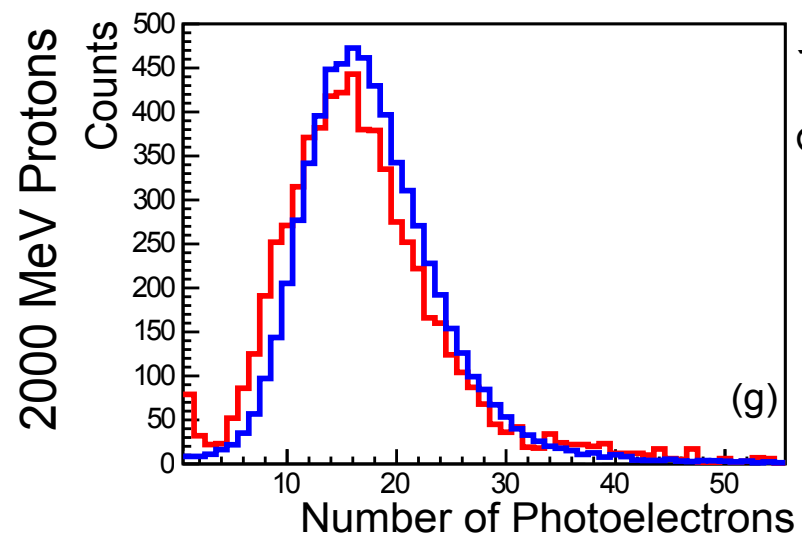
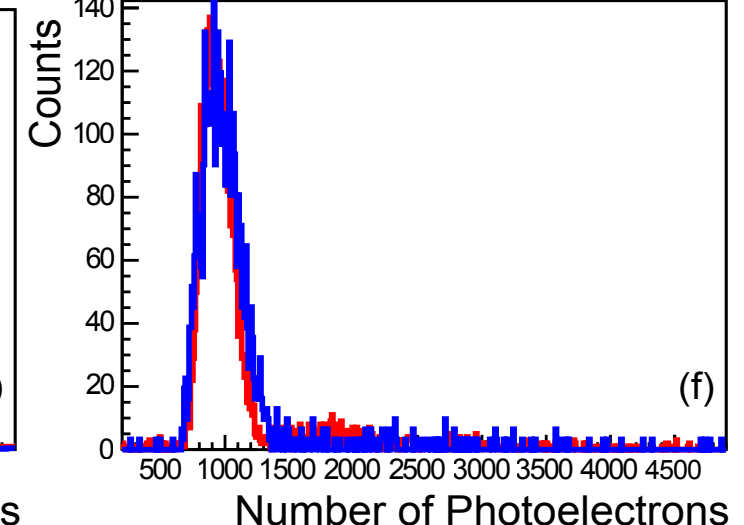
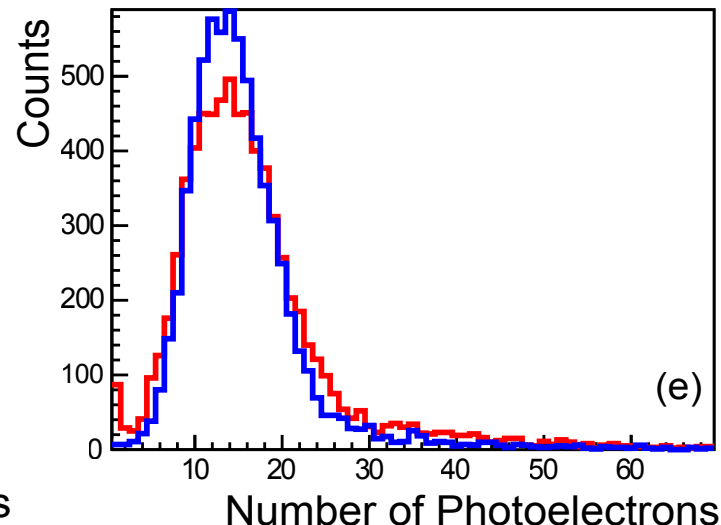
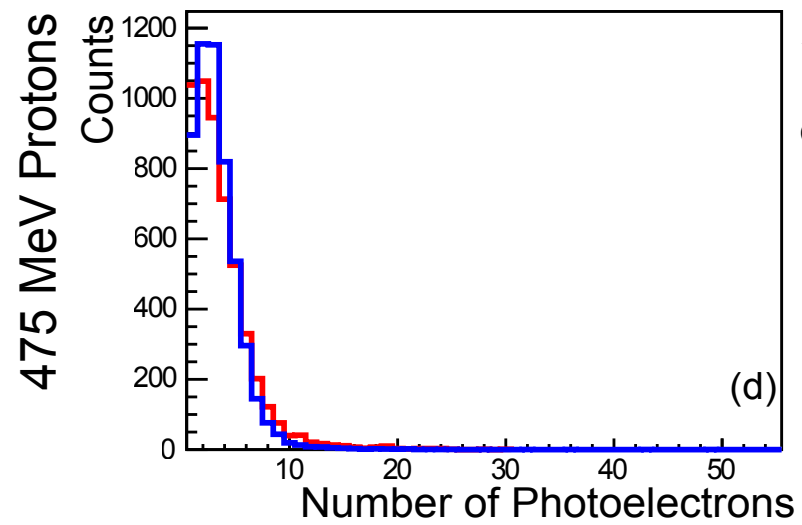
WBLS-2

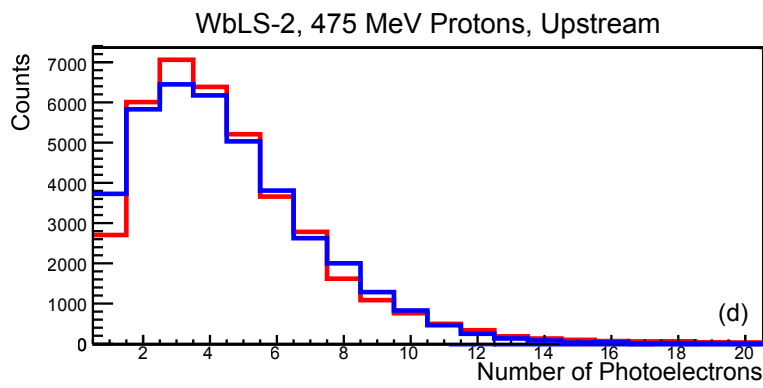
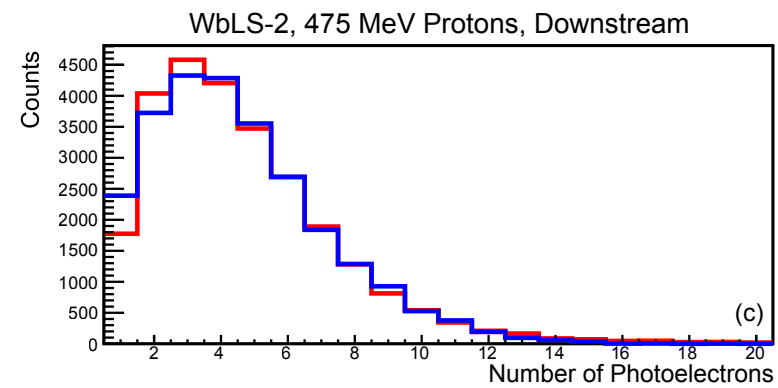
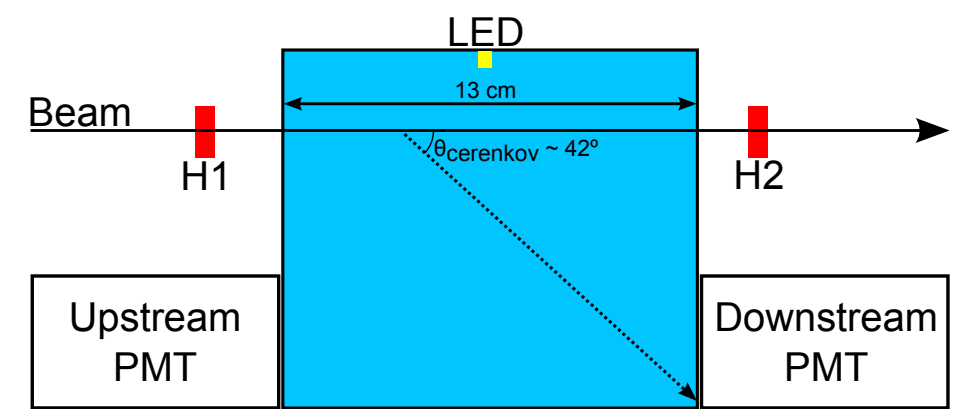
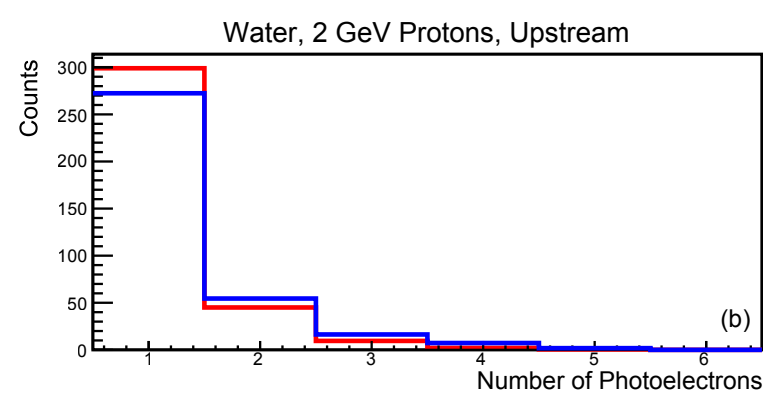
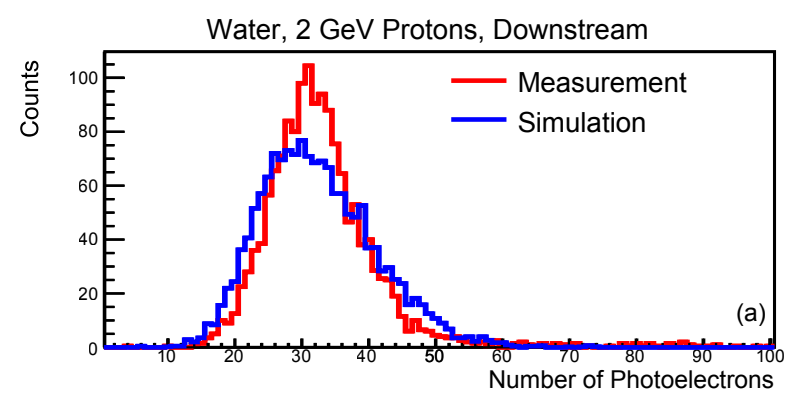


LS

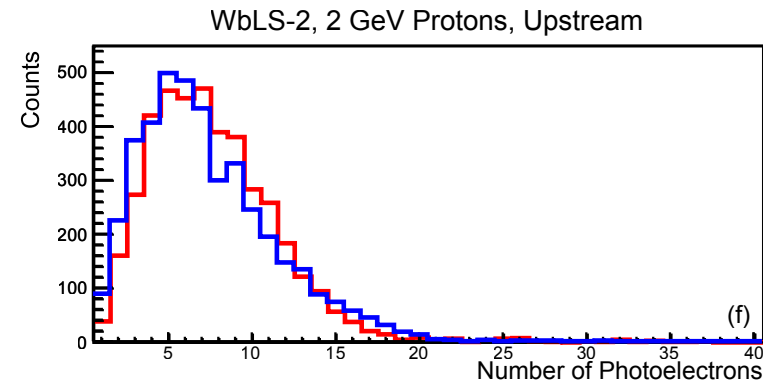
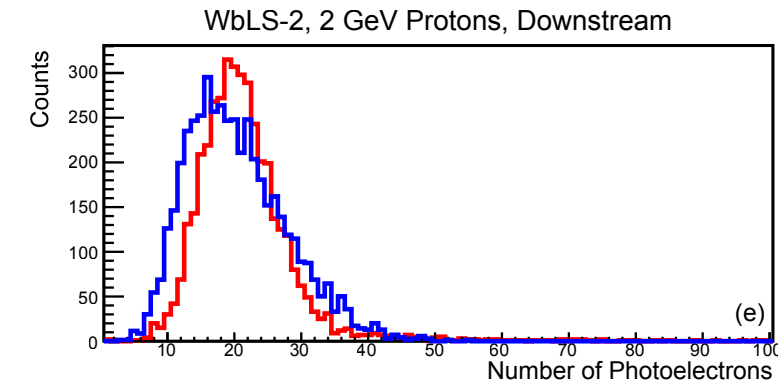


Beam energy





# Comparison of NSRL13A data with simulation

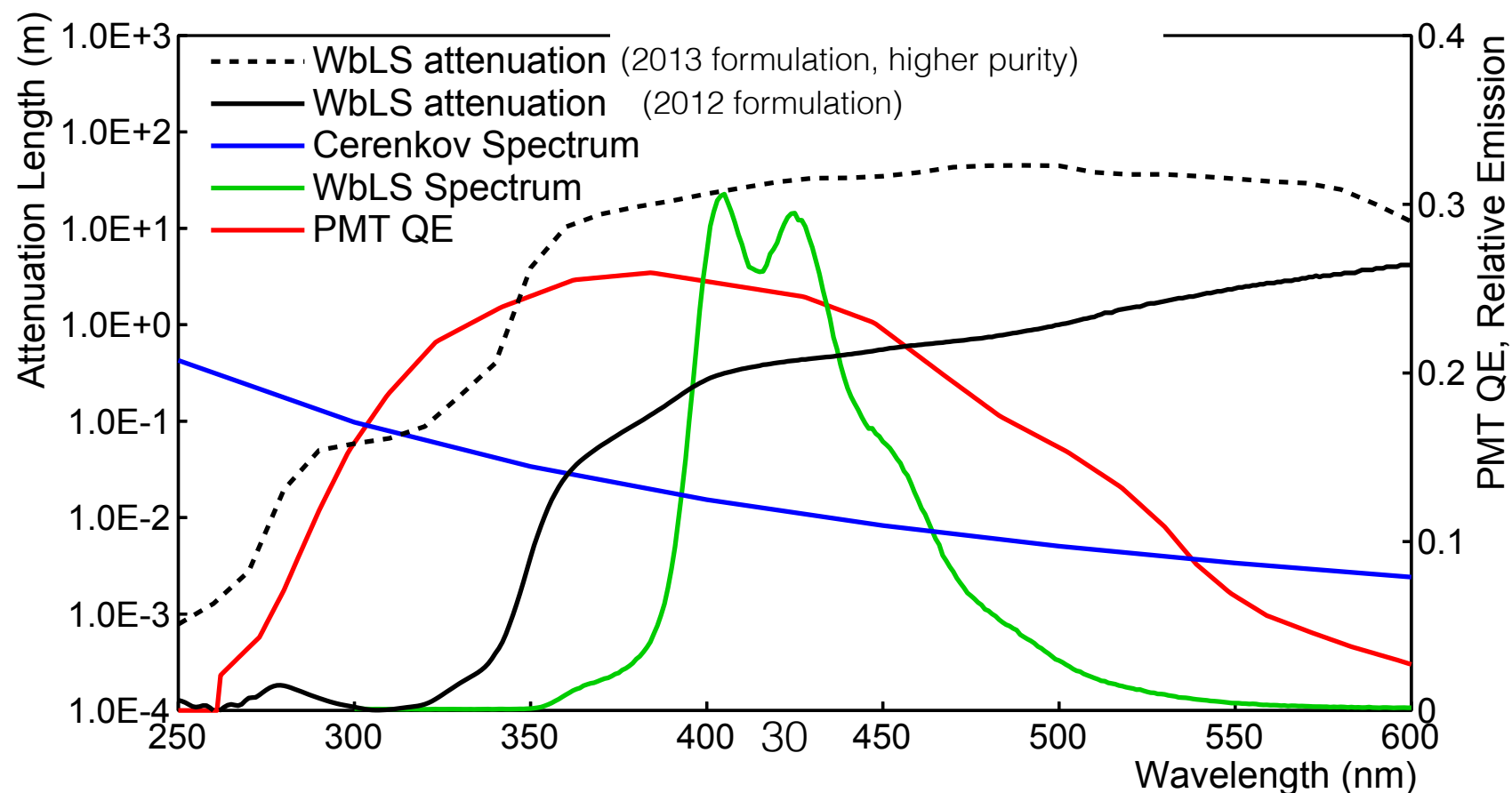


Mean number of  
photoelectrons

Sample	Incident Proton Energy	Photomultiplier	Measured	Simulated
Water	475 MeV	Downstream	$1.3 \pm 0.0$	$1.6 \pm 0.2$
Water	475 MeV	Upstream	$1.2 \pm 0.1$	$1.2 \pm 0.1$
Water	2000 MeV	Downstream	$33.0 \pm 0.2$	$32.4 \pm 3.2$
Water	2000 MeV	Upstream	$1.2 \pm 0.0$	$1.4 \pm 0.1$
WbLS-2	475 MeV	Downstream	$4.7 \pm 0.0$	$4.6 \pm 0.5$
WbLS-2	475 MeV	Upstream	$4.6 \pm 0.0$	$4.5 \pm 0.5$
WbLS-2	2000 MeV	Downstream	$21.5 \pm 0.3$	$20.4 \pm 2.0$
WbLS-2	2000 MeV	Upstream	$7.7 \pm 0.2$	$7.3 \pm 0.7$

# Interplay of Cerenkov and scintillation light

1. Results on previous page indicate that  $1.27 \pm 0.05$  WLS-Cerenkov photons are detected for every detected scintillation photon. [Simulation: 1.28]
2. Absorption probability of detectable Cerenkov light in 1%WbLS at first order is  $\sim 58\%$ . This would be unacceptable for a large detector. Improved WbLS has been developed.





# Light yield and quenching parameters

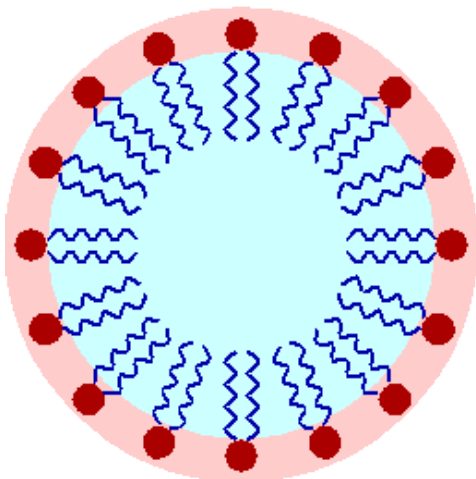
Material	Light yield (photons/MeV)	kB (mm/MeV)
0.4%WbLS	19.9±2.3	0.70±0.14
1%WbLS	109±11	0.44±0.05
LS	9156±917	0.07±0.01

$$\frac{dL}{dx} = L_0 \frac{\frac{dE}{dx}}{1 + kB \frac{dE}{dx}}$$

- LS light yield and kB consistent with other measurements in literature for LS and plastic scintillator ( $0.09 < kB < 0.19$  mm/MeV)
- Light yield of 1% WbLS is ~1% of LS
- kB of WbLS significantly larger than LS.
  - Due to change in bulk LS properties when in emulsion?
  - Due to presence of surfactant and/or water?

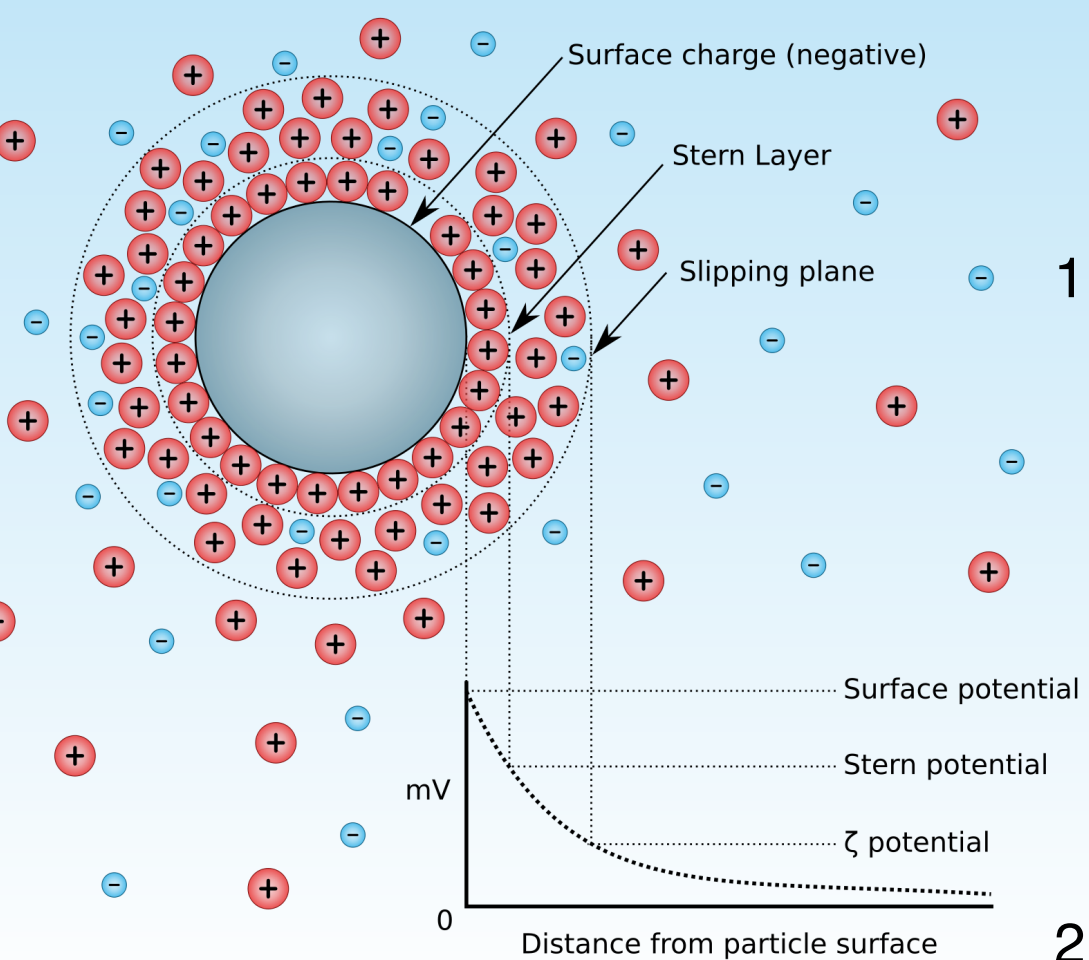
# WbLS is an emulsion

1. A surfactant is added to LS, water mixture to stabilize the emulsion. The surfactant has a hydrophobic “tail” and hydrophilic “head”.
2. A micelle is an aggregate of surfactant molecules dispersed in a liquid colloid. For WbLS, the hydrophilic “head” is in contact with the water, the hydrophobic “tail” sequesters the LS.
3. Absorption length and preliminary diameter measurements suggest micelle diameters of O(10nm).
4. Sequestering the LS to a micelle
  1. Alters the effective diffusion length of the LS molecules which will change the probability of energy transfer and fluorescence decay time.
  2. Allow energy transfer to the surfactant and water affecting light yield/quenching



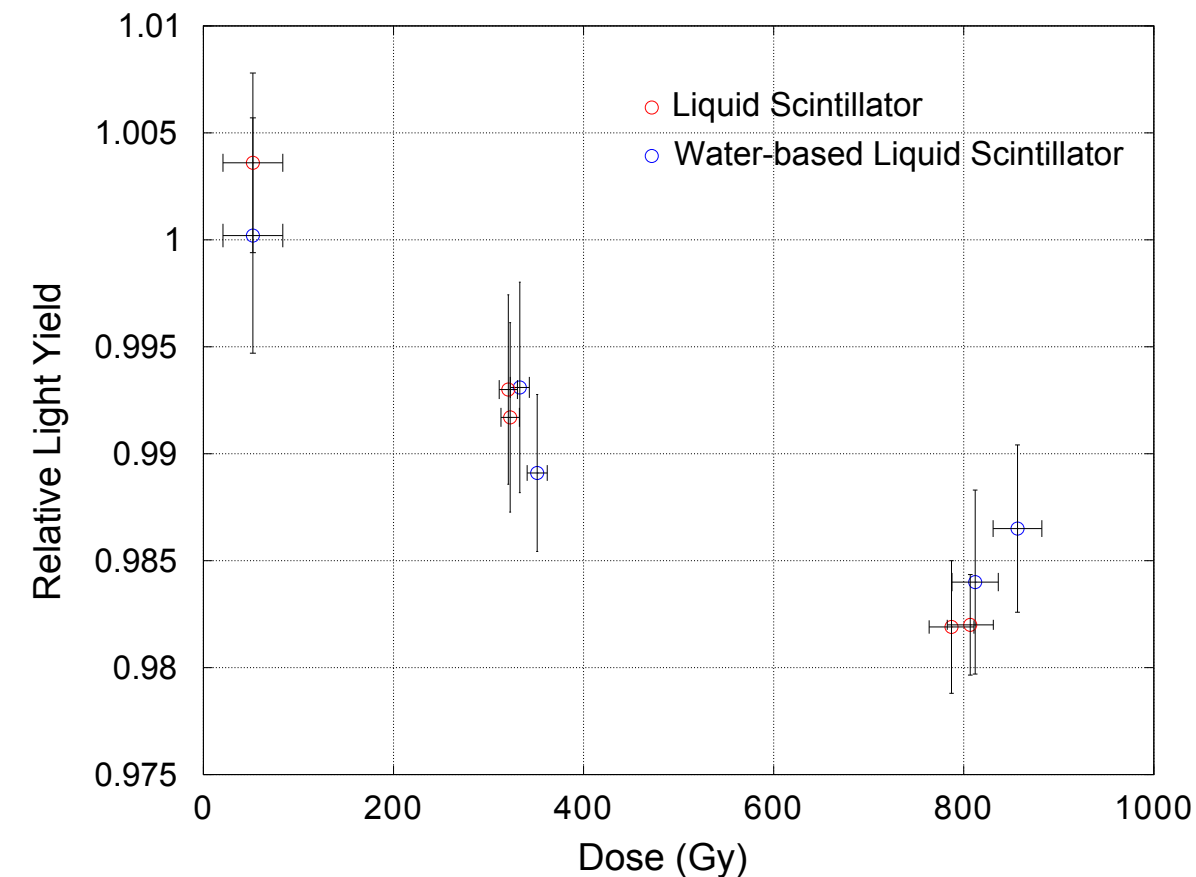
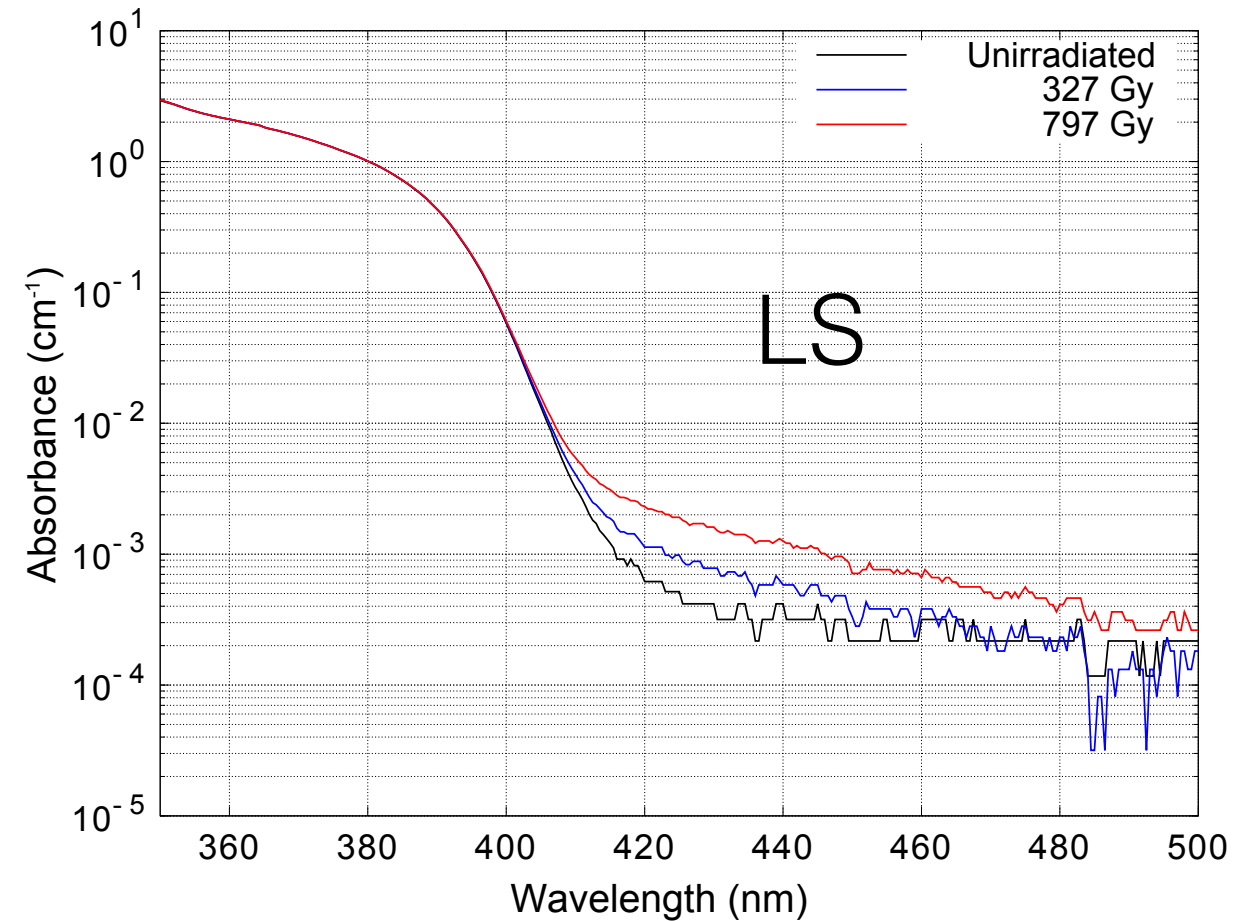
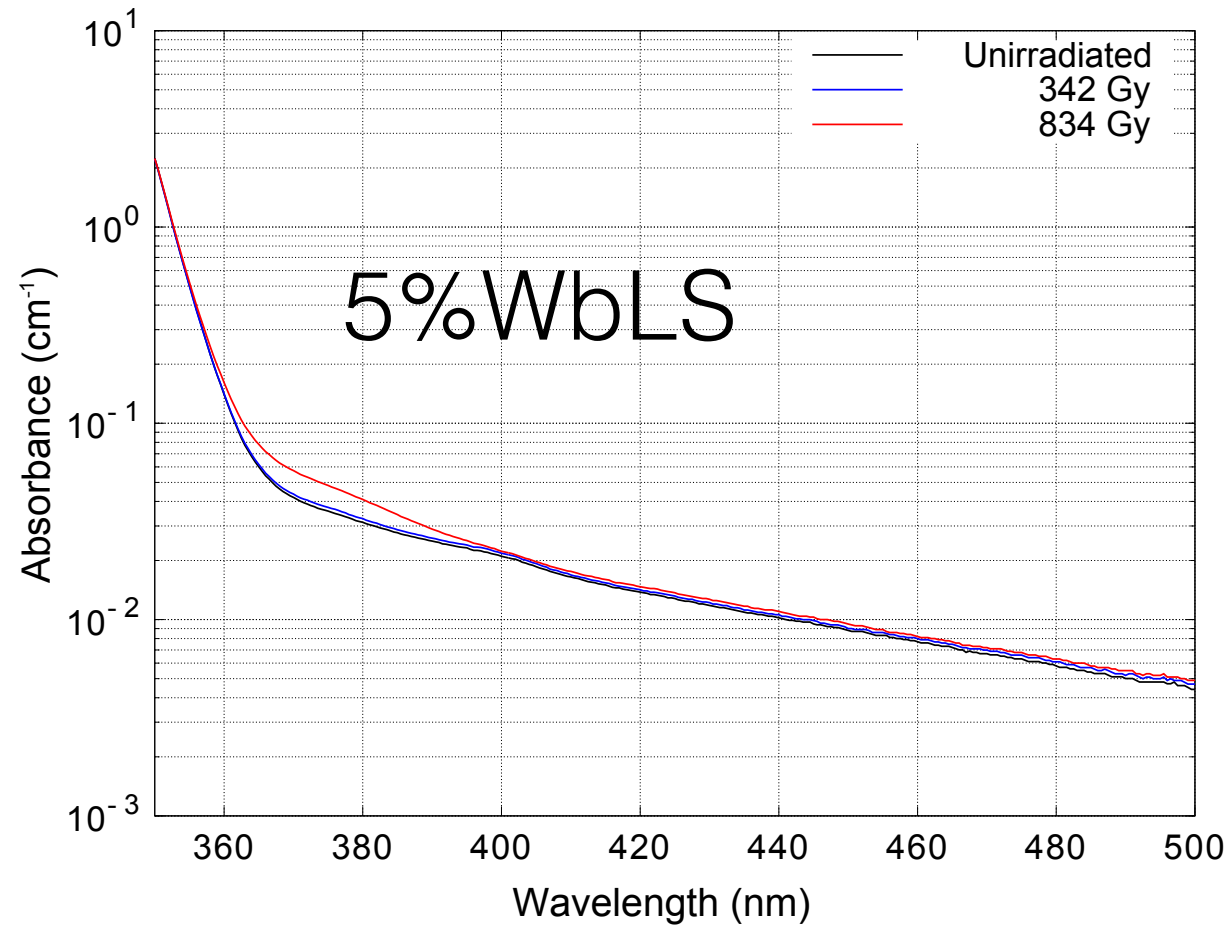
A micelle drawn  
in wikipedia

# WbLS measurements in progress or beginning soon



1. Malvern Zetasizer Nano at BNL Center for Functional Nanomaterials (CFN) will be used to measure micelle size (dynamic light scattering) and  $\zeta$  potential (electrophoretic light scattering)
  1. Micelle sizes affects scattering length, may affect light yield, quenching, decay time.
  2. Emulsion stability improves with increasing  $\zeta$  potential.
2. Fluorescence decay time via Time-Correlated Single Photon Counting, Picoquant FT200TCSPC, at CFN
3. Direct attenuation length measurement with 2-m system (Nucl.Instrum.Meth. A637 (2011) 47-52) in BNL Chemistry.
4. Absolute quantum yield measurement using integrating sphere in BNL Chemistry
5. Quenching and pulse shape discrimination measurements, AmBe and  $^{137}\text{Cs}$  sources, BNL Physics
6. Commissioning a 1000 liter prototype in BNL Physics

# Radiation hardness



1. LY reduced  $1.74 \pm 0.55\%$  and  $1.31 \pm 0.59\%$  for LS, 5%WbLS resp. after  $\sim 800\text{Gy}$  dose at NSRL
2. Implies  $\sim 0.1\%$  LY reduction in one year of operation of a proton therapy QA device



# Summary and prospects

1. Water-based liquid scintillator is a new detection medium invented at BNL with numerous possible applications
2. We have shown that the light yield is adjustable and begun developing a detailed simulation to account for all light production and absorption mechanisms
3. Further investigation underway to understand why WbLS properties differ from bulk LS
4. We are currently commissioning a 1000 liter acrylic vessel to study WbLS performance and characteristics in a modest scale detector
5. We also plan a suite of measurements of light yield, absorbance and emission for various WbLS concentrations to incorporate in simulation

